



wwPDB NMR Structure Validation Summary Report

Jun 3, 2023 – 07:33 PM EDT

PDB ID : 2MRO
Title : Structure of the complex of ubiquitin and the UBA domain from DNA-damage-inducible 1 protein (Ddi1)
Authors : Zhang, D.; Fushman, D.
Deposited on : 2014-07-14

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 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) : 2.33

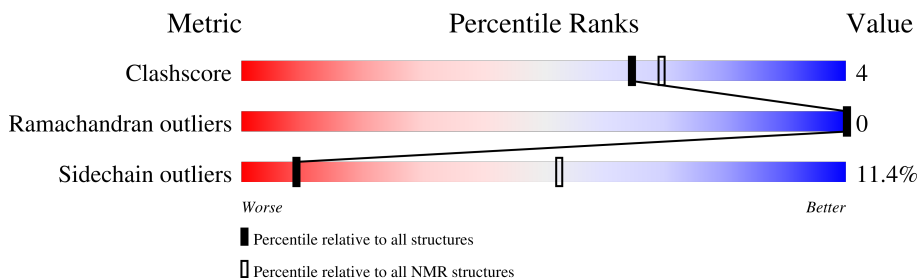
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 13%.

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 | 76 | 87% 11% . |
| 2 | B | 44 | 80% 11% 9% |

2 Ensemble composition and analysis i

This entry contains 10 models. Model 6 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:1-A:74, B:390-B:429 (114) | 0.78 | 6 |

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1156 atoms, of which 220 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polyubiquitin-B.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| | | | Total | C | H | N | O | S | |
| 1 | A | 76 | 746 | 378 | 144 | 105 | 118 | 1 | 0 |

- Molecule 2 is a protein called DNA damage-inducible protein 1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|----|----|----|---|-------|
| | | | Total | C | H | N | O | S | |
| 2 | B | 44 | 410 | 212 | 76 | 56 | 65 | 1 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

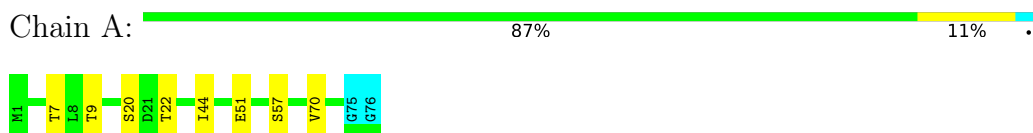
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 386 | GLY | - | expression tag | UNP P40087 |
| B | 387 | SER | - | expression tag | UNP P40087 |
| B | 388 | ALA | - | expression tag | UNP P40087 |
| B | 429 | SER | - | expression tag | UNP P40087 |

4 Residue-property plots [i](#)

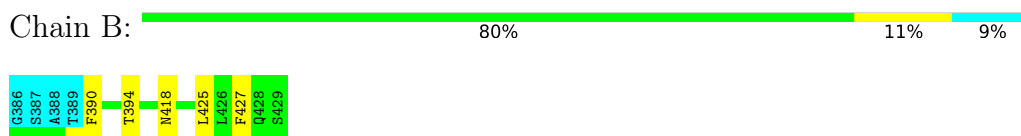
4.1 Average score per residue in the NMR ensemble

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: Polyubiquitin-B



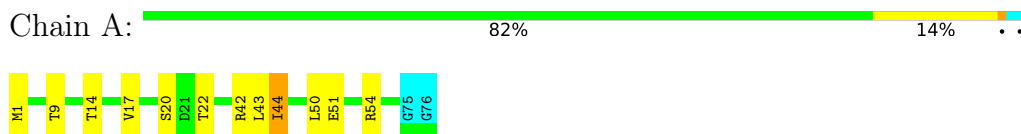
- Molecule 2: DNA damage-inducible protein 1



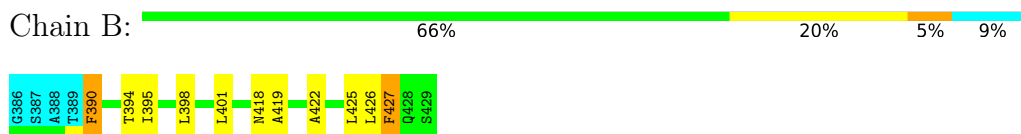
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 6. Colouring as in section 4.1 above.

- Molecule 1: Polyubiquitin-B



- Molecule 2: DNA damage-inducible protein 1



5 Refinement protocol and experimental data overview

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

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| HADDOCK | geometry optimization | 2.1 |
| HADDOCK | refinement | 2.1 |
| HADDOCK | structure solution | 2.1 |

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

| Chemical shift file(s) | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists | 1 |
| Total number of shifts | 210 |
| Number of shifts mapped to atoms | 210 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 13% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 593 | 142 | 623 | 6±2 |
| 2 | B | 312 | 68 | 314 | 4±2 |
| All | All | 9050 | 2100 | 9370 | 78 |

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 4.

5 of 60 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:412:LEU:HD13 | 2:B:417:GLY:HA2 | 0.74 | 1.58 | 3 | 1 |
| 1:A:2:GLN:HE22 | 1:A:16:GLU:HG2 | 0.62 | 1.55 | 8 | 1 |
| 1:A:51:GLU:HB2 | 1:A:54:ARG:HG2 | 0.61 | 1.72 | 7 | 5 |
| 2:B:390:PHE:HB2 | 2:B:395:ILE:HD11 | 0.60 | 1.73 | 3 | 2 |
| 1:A:5:VAL:HB | 1:A:13:ILE:HB | 0.59 | 1.73 | 1 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|------------|------------|-------------|-----|
| 1 | A | 73/76 (96%) | 71±1 (98±1%) | 2±1 (2±1%) | 0±0 (0±0%) | 100 | 100 |
| 2 | B | 39/44 (89%) | 37±1 (96±2%) | 2±1 (4±2%) | 0±0 (0±0%) | 100 | 100 |
| All | All | 1120/1200 (93%) | 1086 (97%) | 34 (3%) | 0 (0%) | 100 | 100 |

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|-------------|-------------|----|
| 1 | A | 68/68 (100%) | 61±2 (89±3%) | 7±2 (11±3%) | 10 | 54 |
| 2 | B | 33/35 (94%) | 29±2 (88±5%) | 4±2 (12±5%) | 8 | 50 |
| All | All | 1010/1030 (98%) | 895 (89%) | 115 (11%) | 9 | 52 |

5 of 37 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 | 22 | THR | 9 |
| 1 | A | 9 | THR | 8 |
| 1 | A | 20 | SER | 7 |
| 1 | A | 7 | THR | 6 |
| 1 | A | 57 | SER | 6 |

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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 13% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [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 | 210 |
| Number of shifts mapped to atoms | 210 |
| 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 |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 0 | — | None (insufficient data) |
| $^{13}\text{C}_\beta$ | 0 | — | None (insufficient data) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 105 | 0.85 ± 0.60 | None needed (imprecise) |

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 13%, i.e. 204 atoms were assigned a chemical shift out of a possible 1606. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 204/566 (36%) | 102/229 (45%) | 0/228 (0%) | 102/109 (94%) |
| Sidechain | 0/964 (0%) | 0/624 (0%) | 0/301 (0%) | 0/39 (0%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 0/76 (0%) | 0/38 (0%) | 0/37 (0%) | 0/1 (0%) |
| Overall | 204/1606 (13%) | 102/891 (11%) | 0/566 (0%) | 102/149 (68%) |

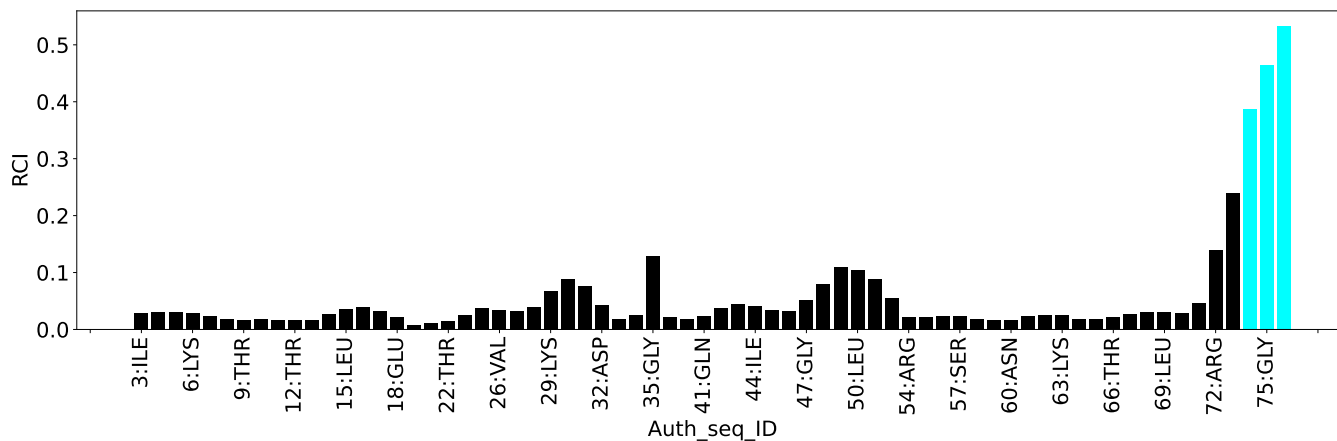
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

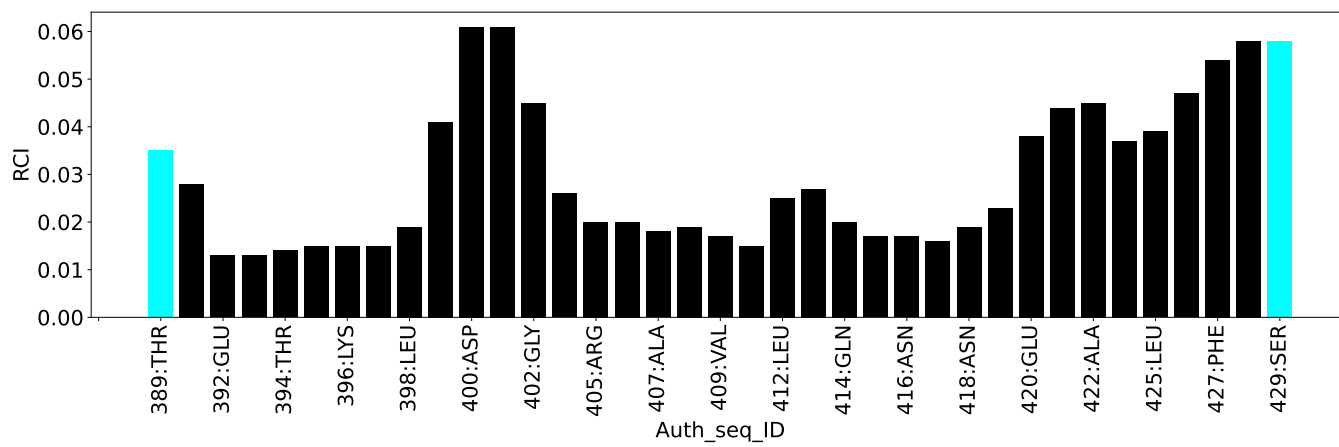
7.1.5 Random Coil Index (RCI) plots [i](#)

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 | 22 |
| Intra-residue ($ i-j =0$) | 0 |
| Sequential ($ i-j =1$) | 0 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 0 |
| Long range ($ i-j \geq 5$) | 0 |
| Inter-chain | 22 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 0.2 |
| Number of long range restraints per residue ¹ | 0.0 |

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

| Bins (Å) | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small) | 2.8 | 0.2 |
| 0.2-0.5 (Medium) | 4.3 | 0.49 |
| >0.5 (Large) | 2.1 | 1.35 |

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

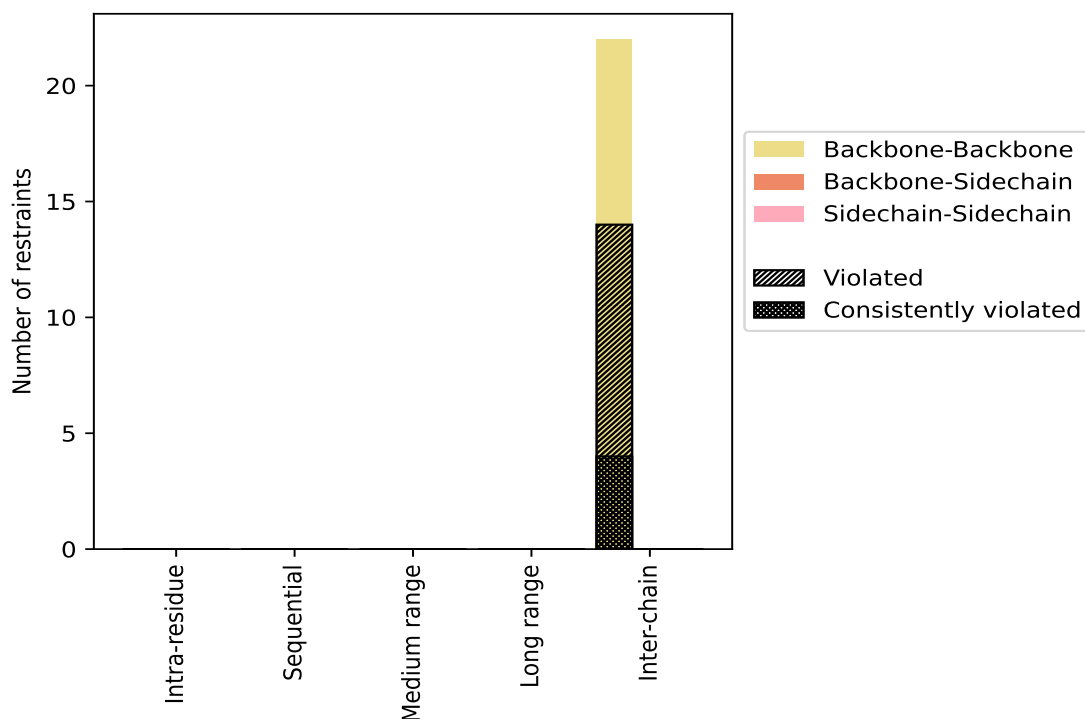
9.1 Summary of distance violations

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) | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sequential (i-j =1) | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Medium range (i-j >1 & i-j <5) | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Long range (i-j ≥5) | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Inter-chain | 22 | 100.0 | 14 | 63.6 | 63.6 | 4 | 18.2 | 18.2 |
| Backbone-Backbone | 22 | 100.0 | 14 | 63.6 | 63.6 | 4 | 18.2 | 18.2 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 22 | 100.0 | 14 | 63.6 | 63.6 | 4 | 18.2 | 18.2 |
| Backbone-Backbone | 22 | 100.0 | 14 | 63.6 | 63.6 | 4 | 18.2 | 18.2 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |

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](#)

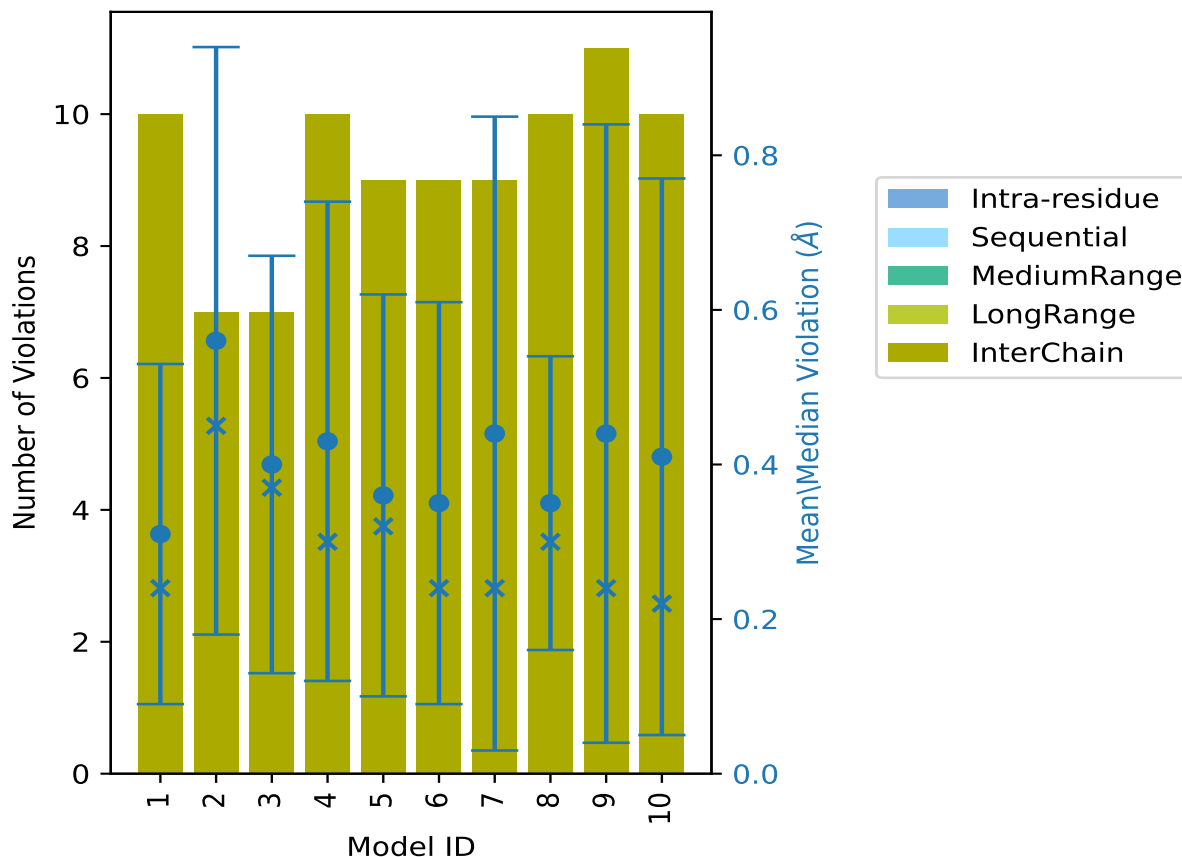
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| 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 | 0 | 0 | 0 | 0 | 10 | 10 | 0.31 | 0.91 | 0.22 | 0.24 |
| 2 | 0 | 0 | 0 | 0 | 7 | 7 | 0.56 | 1.32 | 0.38 | 0.45 |
| 3 | 0 | 0 | 0 | 0 | 7 | 7 | 0.4 | 0.97 | 0.27 | 0.37 |
| 4 | 0 | 0 | 0 | 0 | 10 | 10 | 0.43 | 1.18 | 0.31 | 0.3 |
| 5 | 0 | 0 | 0 | 0 | 9 | 9 | 0.36 | 1.04 | 0.26 | 0.32 |
| 6 | 0 | 0 | 0 | 0 | 9 | 9 | 0.35 | 1.0 | 0.26 | 0.24 |
| 7 | 0 | 0 | 0 | 0 | 9 | 9 | 0.44 | 1.27 | 0.41 | 0.24 |
| 8 | 0 | 0 | 0 | 0 | 10 | 10 | 0.35 | 0.75 | 0.19 | 0.3 |
| 9 | 0 | 0 | 0 | 0 | 11 | 11 | 0.44 | 1.35 | 0.4 | 0.24 |
| 10 | 0 | 0 | 0 | 0 | 10 | 10 | 0.41 | 1.16 | 0.36 | 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, 8(IR:0, SQ:0, MR:0, LR:0, IC:8) 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 | % |
| 0 | 0 | 0 | 0 | 2 | 2 | 1 | 10.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 2 | 20.0 |
| 0 | 0 | 0 | 0 | 1 | 1 | 3 | 30.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 4 | 40.0 |

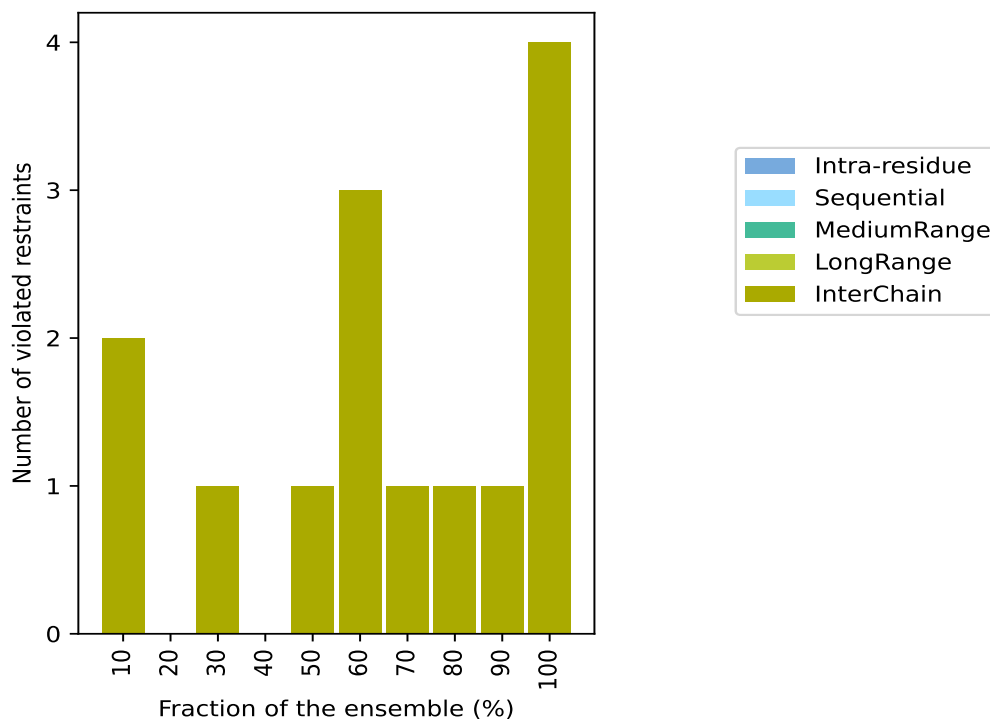
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR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

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

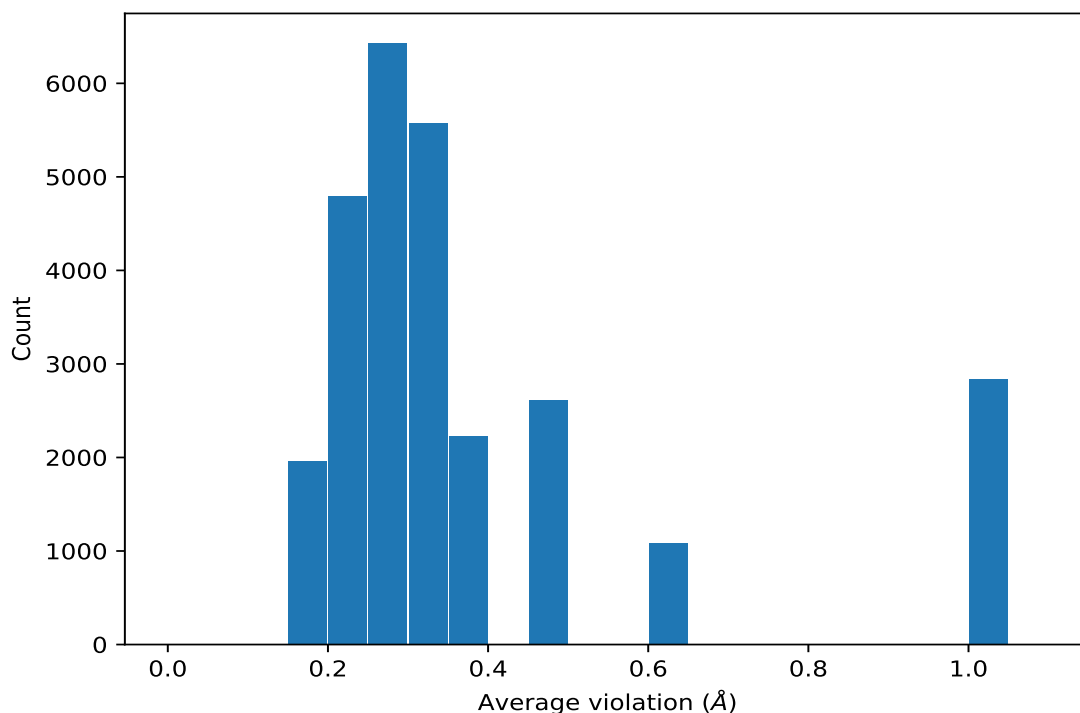
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:SD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CB | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CB | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CE | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ3 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:NZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CG2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:HG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:OG1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD21 | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:ND2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:OD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CB | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CZ | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CD | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:H | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE21 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE22 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:NE2 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:OE1 | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:C | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CA | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CB | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:H | 10 | 1.03 | 0.18 | 1.0 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:HG | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:N | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:O | 10 | 1.03 | 0.18 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:OG | 10 | 1.03 | 0.18 | 1.0 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:4:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:6:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:7:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:8:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:9:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:10:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:10:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:10:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:10:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:10:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:11:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:12:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:C | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:34:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:36:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:37:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:37:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:37:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:37:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:37:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:37:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:37:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:38:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:38:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:38:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:38:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:38:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:38:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:38:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:39:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:C | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:40:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:41:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:42:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:44:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:45:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:46:ALA:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:46:ALA:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:46:ALA:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:46:ALA:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:46:ALA:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:46:ALA:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:47:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:47:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:47:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:47:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:47:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:C | 1:A:48:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:49:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:50:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:51:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:58:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:C | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:HH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:59:TYR:OH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:HD21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:HD22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:ND2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:60:ASN:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:61:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:66:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:HE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:ND1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:68:HIS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:70:VAL:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:70:VAL:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:70:VAL:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:70:VAL:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:70:VAL:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:70:VAL:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:70:VAL:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:70:VAL:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:71:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:72:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:73:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:74:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:75:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:75:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:75:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:75:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:75:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:76:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:76:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:76:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:76:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:C | 1:A:76:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:4:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:6:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:7:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:8:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:C | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:9:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:10:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:10:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:10:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:10:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:10:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:11:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:12:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:34:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:36:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:37:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:37:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:37:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:37:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:37:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:37:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:37:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:38:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:38:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:38:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:38:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:38:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:38:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:38:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:39:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:40:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:41:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:42:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:44:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:45:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:46:ALA:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:46:ALA:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:46:ALA:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:46:ALA:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:46:ALA:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:46:ALA:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:47:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:47:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:47:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:47:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:47:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:48:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:49:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:50:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:51:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:58:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:CE2 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:HH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:59:TYR:OH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:HD21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:HD22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:ND2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:60:ASN:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:61:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:66:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:CG | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:HE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:ND1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:68:HIS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:70:VAL:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:70:VAL:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:70:VAL:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:70:VAL:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:70:VAL:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:70:VAL:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:70:VAL:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:70:VAL:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:71:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:72:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:73:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:74:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:75:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:75:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:75:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:75:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:75:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:76:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:76:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:76:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:76:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CA | 1:A:76:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:4:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:6:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:7:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:8:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:9:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:10:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:10:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:10:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:10:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:10:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:11:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:12:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:34:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:36:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:37:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:37:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:37:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:37:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:37:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:37:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:37:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:38:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:38:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:38:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:38:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:38:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:38:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:38:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:39:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:40:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:C | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:41:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:42:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:44:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:45:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:46:ALA:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:46:ALA:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:46:ALA:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:46:ALA:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:46:ALA:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:46:ALA:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:47:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:47:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:47:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:47:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:47:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:48:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:O | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:49:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:50:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:51:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:58:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:HH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:O | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:59:TYR:OH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:HD21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:HD22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:ND2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:60:ASN:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:61:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:66:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:HE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:ND1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:68:HIS:O | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:70:VAL:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:70:VAL:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:70:VAL:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:70:VAL:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:70:VAL:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:70:VAL:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:70:VAL:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:70:VAL:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:71:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:72:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:CB | 1:A:73:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:74:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:75:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:75:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:75:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:75:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:75:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:76:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:76:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:76:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:76:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:CB | 1:A:76:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:4:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:6:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:7:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:8:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:9:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:10:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:10:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:10:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:10:GLY:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:10:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:11:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:12:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:34:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:36:ILE:O | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:37:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:37:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:37:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:37:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:37:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:37:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:37:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:38:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:38:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:38:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:38:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:38:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:38:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:38:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:39:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:40:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:41:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:42:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:44:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:45:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:46:ALA:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:46:ALA:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:46:ALA:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:46:ALA:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:46:ALA:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:46:ALA:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:47:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:47:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:47:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:47:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:47:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:48:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:49:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:50:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:51:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:58:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:HH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:59:TYR:OH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:H | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:HD21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:HD22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:ND2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:60:ASN:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:61:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:66:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:HE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:ND1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:68:HIS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:70:VAL:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:70:VAL:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:70:VAL:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:70:VAL:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:70:VAL:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:70:VAL:H | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:70:VAL:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:70:VAL:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:71:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:72:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:73:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:74:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:75:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:75:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:75:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:75:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:75:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:76:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:76:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:76:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:76:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:H | 1:A:76:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:4:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:6:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:7:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:8:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:9:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:10:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:10:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:10:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:10:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:10:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:11:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:12:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:34:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:36:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:37:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:37:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:37:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:37:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:37:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:37:PRO:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:37:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:38:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:38:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:38:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:38:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:38:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:38:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:38:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:39:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:40:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:41:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:C | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:42:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:44:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:45:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:46:ALA:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:46:ALA:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:46:ALA:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:46:ALA:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:46:ALA:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:46:ALA:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:47:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:47:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:47:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:47:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:47:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:48:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:49:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:50:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:51:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:58:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:HH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:59:TYR:OH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:HD21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:HD22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:ND2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:60:ASN:OD1 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:61:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:66:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:HE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:ND1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:68:HIS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:70:VAL:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:70:VAL:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:70:VAL:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:70:VAL:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:70:VAL:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:70:VAL:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:70:VAL:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:70:VAL:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:71:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:72:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:73:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:74:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:75:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:75:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:75:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:75:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:75:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:76:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:76:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:76:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:76:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:N | 1:A:76:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:4:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:6:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:C | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:7:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:8:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:9:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:10:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:10:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:10:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:10:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:10:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:N | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:11:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:12:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:34:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:36:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:37:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:37:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:37:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:37:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:37:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:37:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:37:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:38:PRO:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:38:PRO:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:38:PRO:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:38:PRO:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:38:PRO:CG | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:38:PRO:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:38:PRO:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:39:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:40:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:41:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:H | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:42:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:44:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:45:PHE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:46:ALA:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:46:ALA:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:46:ALA:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:46:ALA:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:46:ALA:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:46:ALA:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:47:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:47:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:47:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:47:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:47:GLY:O | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:CE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:HZ1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:HZ2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:HZ3 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:NZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:48:LYS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:HE21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:HE22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:49:GLN:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:50:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:O | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:OE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:51:GLU:OE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:58:ASP:OD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:CE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:HH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:59:TYR:OH | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:HD21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:HD22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:ND2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:60:ASN:OD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:CG2 | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:61:ILE:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:HG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:66:THR:OG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:CE1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:HE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:ND1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:NE2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:68:HIS:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:70:VAL:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:70:VAL:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:70:VAL:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:70:VAL:CG1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:70:VAL:CG2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:70:VAL:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:70:VAL:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:70:VAL:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:71:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:C | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:72:ARG:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:CD1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:CD2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:73:LEU:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:CB | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:CD | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:CG | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:CZ | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:HE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:HH11 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:HH12 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:HH21 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:HH22 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:NE | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:NH1 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:NH2 | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:74:ARG:O | 10 | 0.39 | 0.13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,17) | 2:B:423:ALA:O | 1:A:75:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:75:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:75:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:75:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:75:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:76:GLY:C | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:76:GLY:CA | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:76:GLY:H | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:76:GLY:N | 10 | 0.39 | 0.13 | 0.41 |
| (1,17) | 2:B:423:ALA:O | 1:A:76:GLY:O | 10 | 0.39 | 0.13 | 0.41 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:C | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:C | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CA | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CA | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CB | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CD | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CD | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:CG | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:H | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:N | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:N | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|---------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:O | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:O | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE1 | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE1 | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|---------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:4:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:6:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:7:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:8:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:C | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:9:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:10:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:10:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:10:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:10:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:10:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:11:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:12:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:34:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:36:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:37:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:37:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:37:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:37:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:37:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:37:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:37:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:38:PRO:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:38:PRO:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:38:PRO:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:38:PRO:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:38:PRO:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:38:PRO:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:38:PRO:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:39:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:40:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:41:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:42:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:N | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:44:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:CE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:45:PHE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:46:ALA:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:46:ALA:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:46:ALA:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:46:ALA:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:46:ALA:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:46:ALA:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:47:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:47:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:47:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:47:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:47:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:CE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:HZ1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:HZ2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:HZ3 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:NZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:48:LYS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:HE21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:HE22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:49:GLN:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:50:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:OE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:51:GLU:OE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:58:ASP:OD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:CE2 | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:HH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:59:TYR:OH | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:HD21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:HD22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:ND2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:60:ASN:OD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:61:ILE:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:HG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:66:THR:OG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:CE1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:CG | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:HE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:ND1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:NE2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:68:HIS:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:70:VAL:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:70:VAL:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:70:VAL:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:70:VAL:CG1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:70:VAL:CG2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:70:VAL:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:70:VAL:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:70:VAL:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:71:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:72:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:CA | 10 | 0.35 | 0.21 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:CD1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:CD2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:73:LEU:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:CB | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:CD | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:CG | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:CZ | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:HE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:HH11 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:HH12 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:HH21 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:HH22 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:NE | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:NH1 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:NH2 | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:74:ARG:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:75:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:75:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:75:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:75:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:75:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:76:GLY:C | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:76:GLY:CA | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:76:GLY:H | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:76:GLY:N | 10 | 0.35 | 0.21 | 0.26 |
| (1,16) | 2:B:420:GLU:OE2 | 1:A:76:GLY:O | 10 | 0.35 | 0.21 | 0.26 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:4:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:6:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:7:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:8:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:9:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:10:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:10:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:10:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:10:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:10:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:11:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:12:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:34:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:36:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:37:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:37:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:37:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:37:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:37:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:37:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:37:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:38:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:38:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:38:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:38:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:38:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:38:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:38:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:39:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:40:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:C | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:41:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:42:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:44:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:45:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:46:ALA:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:46:ALA:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:46:ALA:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:46:ALA:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:46:ALA:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:46:ALA:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:47:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:47:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:47:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:47:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:47:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:48:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:O | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:49:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:50:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:51:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:58:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:HH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:O | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:59:TYR:OH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:HD21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:HD22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:ND2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:60:ASN:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:61:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:66:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:HE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:ND1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:68:HIS:O | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:70:VAL:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:70:VAL:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:70:VAL:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:70:VAL:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:70:VAL:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:70:VAL:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:70:VAL:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:70:VAL:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:71:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:72:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:C | 1:A:73:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:74:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:75:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:75:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:75:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:75:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:75:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:76:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:76:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:76:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:76:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:C | 1:A:76:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:4:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:6:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:7:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:8:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:9:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:10:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:10:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:10:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:10:GLY:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:10:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:11:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:12:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:34:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:36:ILE:O | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:37:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:37:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:37:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:37:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:37:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:37:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:37:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:38:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:38:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:38:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:38:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:38:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:38:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:38:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:39:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:40:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:41:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:42:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:44:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:45:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:46:ALA:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:46:ALA:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:46:ALA:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:46:ALA:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:46:ALA:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:46:ALA:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:47:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:47:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:47:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:47:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:47:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:48:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:49:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:50:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:51:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:58:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:HH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:59:TYR:OH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:H | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:HD21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:HD22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:ND2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:60:ASN:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:61:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:66:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:HE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:ND1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:68:HIS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:70:VAL:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:70:VAL:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:70:VAL:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:70:VAL:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:70:VAL:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:70:VAL:H | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:70:VAL:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:70:VAL:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:71:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:72:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:73:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:74:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:75:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:75:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:75:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:75:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:75:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:76:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:76:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:76:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:76:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:CA | 1:A:76:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:4:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:6:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:7:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:8:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:9:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:10:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:10:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:10:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:10:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:10:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:11:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:12:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:34:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:36:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:37:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:37:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:37:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:37:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:37:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:37:PRO:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:37:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:38:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:38:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:38:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:38:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:38:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:38:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:38:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:39:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:40:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:41:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:C | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:42:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:44:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:45:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:46:ALA:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:46:ALA:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:46:ALA:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:46:ALA:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:46:ALA:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:46:ALA:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:47:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:47:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:47:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:47:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:47:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:48:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:49:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:50:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:51:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:58:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:HH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:59:TYR:OH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:HD21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:HD22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:ND2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:60:ASN:OD1 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:61:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:66:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:HE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:ND1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:68:HIS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:70:VAL:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:70:VAL:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:70:VAL:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:70:VAL:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:70:VAL:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:70:VAL:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:70:VAL:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:70:VAL:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:71:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:72:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:73:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:74:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:75:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:75:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:75:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:75:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:75:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:76:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:76:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:76:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:76:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:H | 1:A:76:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:4:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:6:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:C | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:7:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:8:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:9:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:10:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:10:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:10:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:10:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:10:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:11:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:12:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:34:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:36:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:37:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:37:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:37:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:37:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:37:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:37:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:37:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:38:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:38:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:38:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:38:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:38:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:38:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:38:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:39:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:40:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:41:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:H | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:42:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:44:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:45:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:46:ALA:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:46:ALA:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:46:ALA:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:46:ALA:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:46:ALA:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:46:ALA:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:47:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:47:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:47:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:47:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:47:GLY:O | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:48:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:49:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:50:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:O | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:51:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:58:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:HH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:59:TYR:OH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:HD21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:HD22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:ND2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:60:ASN:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:61:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:66:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:HE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:ND1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:68:HIS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:70:VAL:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:70:VAL:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:70:VAL:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:70:VAL:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:70:VAL:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:70:VAL:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:70:VAL:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:70:VAL:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:71:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:C | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:72:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:73:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:74:ARG:O | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:N | 1:A:75:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:75:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:75:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:75:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:75:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:76:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:76:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:76:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:76:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:N | 1:A:76:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:4:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:6:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:7:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:8:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:9:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:10:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:10:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:10:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:10:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:10:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:11:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:12:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:34:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:36:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:37:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:37:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:37:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:37:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:37:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:37:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:37:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:38:PRO:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:38:PRO:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:38:PRO:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:38:PRO:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:38:PRO:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:38:PRO:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:38:PRO:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:39:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:40:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:41:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:N | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:42:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:44:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:45:PHE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:46:ALA:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:46:ALA:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:46:ALA:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:46:ALA:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:46:ALA:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:46:ALA:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:47:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:47:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:47:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:47:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:47:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:CE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:CG | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:HZ1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:HZ2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:HZ3 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:NZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:48:LYS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:HE21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:HE22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:49:GLN:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:50:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:OE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:51:GLU:OE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:CG | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:58:ASP:OD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:CE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:HH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:59:TYR:OH | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:HD21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:HD22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:ND2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:60:ASN:OD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:61:ILE:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:CB | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:HG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:66:THR:OG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:CE1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:HE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:ND1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:NE2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:68:HIS:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:70:VAL:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:70:VAL:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:70:VAL:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:70:VAL:CG1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:70:VAL:CG2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:70:VAL:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:70:VAL:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:70:VAL:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:71:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:H | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:72:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:CD1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:CD2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:73:LEU:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:CB | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:CD | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:CG | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:CZ | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:HE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:HH11 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:HH12 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:HH21 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:HH22 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:NE | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:NH1 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:NH2 | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:74:ARG:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:75:GLY:C | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:75:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:75:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:75:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:75:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:76:GLY:C | 10 | 0.32 | 0.13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,15) | 2:B:402:GLY:O | 1:A:76:GLY:CA | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:76:GLY:H | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:76:GLY:N | 10 | 0.32 | 0.13 | 0.25 |
| (1,15) | 2:B:402:GLY:O | 1:A:76:GLY:O | 10 | 0.32 | 0.13 | 0.25 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:C | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:C | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:C | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:C | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CA | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CB | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CB | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CD1 | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CD1 | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG1 | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG1 | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG1 | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG2 | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG2 | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:CG2 | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:H | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:N | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:N | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:394:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:H | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:396:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:397:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:399:MET:SD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:400:ASP:OD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:401:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:402:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:402:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:402:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:402:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:402:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:403:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:404:PRO:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:404:PRO:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:404:PRO:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:404:PRO:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:404:PRO:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:404:PRO:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:404:PRO:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:CE | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:HZ1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:HZ2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:HZ3 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:NZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:410:LYS:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:414:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:CG2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:HG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:415:THR:OG1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:417:GLY:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:417:GLY:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:417:GLY:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:417:GLY:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:417:GLY:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:HD21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:HD22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:ND2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:418:ASN:OD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:419:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:419:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:419:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:419:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:419:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:419:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:C | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:420:GLU:OE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:421:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:423:ALA:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:423:ALA:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:423:ALA:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:423:ALA:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:423:ALA:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:423:ALA:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:424:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:424:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:424:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:424:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:424:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:424:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:424:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:424:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:H | 9 | 0.19 | 0.06 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:425:LEU:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:CD1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:CD2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:CE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:CE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:CZ | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:427:PHE:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:CD | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:CG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:HE21 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:HE22 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:NE2 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:428:GLN:OE1 | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:429:SER:C | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:429:SER:CA | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:429:SER:CB | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:429:SER:H | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:429:SER:HG | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:429:SER:N | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:429:SER:O | 9 | 0.19 | 0.06 | 0.15 |
| (1,5) | 1:A:44:ILE:O | 2:B:429:SER:OG | 9 | 0.19 | 0.06 | 0.15 |
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:C | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:C | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:C | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:C | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CA | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CA | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CA | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CA | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CA | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CB | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CB | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD1 | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD2 | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CD2 | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CG | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:CG | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:H | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:H | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:H | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:N | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:N | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:N | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:N | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:394:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:396:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:H | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:397:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:399:MET:SD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:400:ASP:OD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:401:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:402:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:402:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:402:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:402:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:402:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:403:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:404:PRO:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:404:PRO:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:404:PRO:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:404:PRO:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:404:PRO:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:404:PRO:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:404:PRO:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:CE | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:HZ1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:HZ2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:HZ3 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:NZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:410:LYS:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:414:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:CA | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:CG2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:HG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:415:THR:OG1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:417:GLY:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:417:GLY:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:417:GLY:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:417:GLY:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:417:GLY:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:HD21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:HD22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:ND2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:418:ASN:OD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:419:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:419:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:419:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:419:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:419:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:419:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:420:GLU:OE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:421:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:423:ALA:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:423:ALA:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:423:ALA:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:423:ALA:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:423:ALA:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:423:ALA:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:424:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:424:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:424:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:424:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:424:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:424:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:424:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:424:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:425:LEU:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:CD1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:CD2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:CE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:CE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:CZ | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:H | 8 | 0.25 | 0.13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:427:PHE:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:CD | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:CG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:HE21 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:HE22 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:NE2 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:428:GLN:OE1 | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:429:SER:C | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:429:SER:CA | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:429:SER:CB | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:429:SER:H | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:429:SER:HG | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:429:SER:N | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:429:SER:O | 8 | 0.25 | 0.13 | 0.22 |
| (1,11) | 1:A:71:LEU:O | 2:B:429:SER:OG | 8 | 0.25 | 0.13 | 0.22 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:394:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:N | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:396:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:397:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:399:MET:SD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:400:ASP:OD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:401:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:402:GLY:C | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:C | 2:B:402:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:402:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:402:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:402:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:403:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:404:PRO:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:404:PRO:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:404:PRO:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:404:PRO:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:404:PRO:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:404:PRO:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:404:PRO:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:410:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:H | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:414:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:415:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:417:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:417:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:417:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:417:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:417:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:HD21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:HD22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:ND2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:418:ASN:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:419:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:419:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:419:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:419:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:419:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:419:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:CG | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:420:GLU:OE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:421:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:423:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:423:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:423:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:423:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:423:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:423:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:424:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:424:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:424:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:424:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:424:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:424:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:424:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:424:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:425:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:427:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:428:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:429:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:429:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:429:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:429:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:429:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:429:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:429:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:C | 2:B:429:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:394:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:396:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:397:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:399:MET:SD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:400:ASP:OD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:401:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:402:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:402:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:402:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:402:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:402:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:403:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:404:PRO:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:404:PRO:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:404:PRO:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:404:PRO:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:404:PRO:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:404:PRO:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:404:PRO:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:N | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:410:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:414:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:415:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:417:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:417:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:417:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:417:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:417:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:HD21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:HD22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:ND2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:418:ASN:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:419:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:419:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:419:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CA | 2:B:419:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:419:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:419:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:420:GLU:OE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:421:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:423:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:423:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:423:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:423:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:423:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:423:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:424:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:424:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:424:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:424:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:424:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:424:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:424:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:424:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:425:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:427:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:428:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:429:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:429:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:429:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:429:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:429:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:429:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:429:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CA | 2:B:429:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:394:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:396:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:397:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:399:MET:SD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:CB | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:400:ASP:OD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:401:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:402:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:402:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:402:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:402:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:402:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:403:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:404:PRO:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:404:PRO:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:404:PRO:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:404:PRO:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:404:PRO:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:404:PRO:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:404:PRO:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:410:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:414:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:415:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:417:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:417:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:417:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:417:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:417:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:HD21 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:HD22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:ND2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:418:ASN:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:419:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:419:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:419:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:419:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:419:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:419:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:420:GLU:OE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:421:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:423:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:423:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:423:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:423:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:423:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:423:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:424:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:424:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:424:SER:CB | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CB | 2:B:424:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:424:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:424:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:424:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:424:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:425:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:427:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:428:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:429:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:429:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:429:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:429:SER:H | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CB | 2:B:429:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:429:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:429:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CB | 2:B:429:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:394:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:396:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:397:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:CE | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:399:MET:SD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:400:ASP:OD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:401:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:402:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:402:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:402:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:402:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:402:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:403:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:404:PRO:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:404:PRO:CA | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG1 | 2:B:404:PRO:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:404:PRO:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:404:PRO:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:404:PRO:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:404:PRO:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:410:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:414:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:415:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:417:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:417:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:417:GLY:H | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG1 | 2:B:417:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:417:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:HD21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:HD22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:ND2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:418:ASN:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:419:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:419:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:419:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:419:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:419:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:419:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:420:GLU:OE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:421:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:423:ALA:C | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG1 | 2:B:423:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:423:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:423:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:423:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:423:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:424:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:424:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:424:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:424:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:424:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:424:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:424:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:424:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:425:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:427:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:428:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:429:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:429:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:429:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:429:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:429:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:429:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:429:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG1 | 2:B:429:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:394:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:396:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:397:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:399:MET:SD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:400:ASP:OD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:401:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:402:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:402:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:402:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:402:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:402:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:403:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:404:PRO:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:404:PRO:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:404:PRO:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:404:PRO:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:404:PRO:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:404:PRO:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:404:PRO:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:410:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:414:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:415:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:417:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:417:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:417:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:417:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:417:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:HD21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:HD22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:ND2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:418:ASN:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:419:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:419:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:419:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:419:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:419:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:419:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:420:GLU:OE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:421:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:423:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:423:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:423:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:423:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:423:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:423:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:424:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:424:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:424:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:424:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:424:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:424:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:424:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:424:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:425:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:427:PHE:O | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:428:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:429:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:429:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:429:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:429:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:429:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:429:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:429:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:CG2 | 2:B:429:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:394:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:396:LYS:O | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:397:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:399:MET:SD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:400:ASP:OD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:401:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:402:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:402:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:402:GLY:H | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:H | 2:B:402:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:402:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:403:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:404:PRO:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:404:PRO:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:404:PRO:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:404:PRO:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:404:PRO:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:404:PRO:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:404:PRO:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:410:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:414:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:415:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:417:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:417:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:417:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:417:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:417:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:HD21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:HD22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:ND2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:418:ASN:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:419:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:419:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:419:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:419:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:419:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:419:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:N | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:420:GLU:OE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:421:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:423:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:423:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:423:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:423:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:423:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:423:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:424:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:424:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:424:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:424:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:424:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:424:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:424:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:424:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:425:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:427:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:428:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:429:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:429:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:429:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:429:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:429:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:429:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:429:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:H | 2:B:429:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:394:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:396:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:397:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:399:MET:SD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:400:ASP:OD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:401:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:402:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:402:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:402:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:402:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:402:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:403:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:404:PRO:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:404:PRO:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:404:PRO:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:404:PRO:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:404:PRO:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:404:PRO:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:404:PRO:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:410:LYS:O | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:414:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:415:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:417:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:417:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:417:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:417:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:417:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:HD21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:HD22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:ND2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:418:ASN:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:419:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:419:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:419:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:419:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:419:ALA:N | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:N | 2:B:419:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:420:GLU:OE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:421:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:423:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:423:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:423:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:423:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:423:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:423:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:424:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:424:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:424:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:424:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:424:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:424:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:424:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:424:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:425:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:427:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:428:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:429:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:429:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:429:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:429:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:429:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:429:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:429:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:N | 2:B:429:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:394:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:396:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:397:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:CE | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:399:MET:SD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:H | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:400:ASP:OD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:401:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:402:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:402:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:402:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:402:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:402:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:403:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:404:PRO:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:404:PRO:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:404:PRO:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:404:PRO:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:404:PRO:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:404:PRO:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:404:PRO:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:CE | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:HZ1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:HZ2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:HZ3 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:NZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:410:LYS:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:414:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:CG2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:HG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:415:THR:OG1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:417:GLY:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:417:GLY:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:417:GLY:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:417:GLY:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:417:GLY:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:HD21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:HD22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:N | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:ND2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:418:ASN:OD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:419:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:419:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:419:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:419:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:419:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:419:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:420:GLU:OE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:421:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:423:ALA:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:423:ALA:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:423:ALA:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:423:ALA:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:423:ALA:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:423:ALA:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:424:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:424:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:424:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:424:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:424:SER:HG | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:O | 2:B:424:SER:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:424:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:424:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:425:LEU:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:CD1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:CD2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:CE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:CE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:CZ | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:427:PHE:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:CD | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:CG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:HE21 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:HE22 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:N | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:NE2 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:428:GLN:OE1 | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:429:SER:C | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:429:SER:CA | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:429:SER:CB | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:429:SER:H | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:429:SER:HG | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:429:SER:N | 7 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|--------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:A:70:VAL:O | 2:B:429:SER:O | 7 | 0.23 | 0.07 | 0.24 |
| (1,10) | 1:A:70:VAL:O | 2:B:429:SER:OG | 7 | 0.23 | 0.07 | 0.24 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:H | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:SD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:OD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CD | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:O | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:HD21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:HD22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:ND2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:OE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:SD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:OD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:HD21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:HD22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:ND2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:OE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:SD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:OD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:O | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:HD21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:HD22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:ND2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:OE1 | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:OE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:H | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:SD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:OD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:HD21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:HD22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:ND2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:C | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:OE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:H | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:O | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:SD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:O | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:OD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CE | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:H | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ3 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:NZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CG2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:HG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:OG1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:HD21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:HD22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:ND2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:O | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:OD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:OE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:O | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:OG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CD1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CD2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CZ | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CD | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:HE21 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:HE22 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:NE2 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:OE1 | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:C | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:CA | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:CB | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:H | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:HG | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:N | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:O | 6 | 0.62 | 0.5 | 0.48 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:OG | 6 | 0.62 | 0.5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:C | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:C | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:C | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:C | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:C | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CA | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CA | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CB | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD1 | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD1 | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD2 | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|---------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CD2 | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CG | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:CG | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:CG | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:H | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:H | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:H | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:H | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:N | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:394:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:N | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:396:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:397:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:399:MET:SD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:400:ASP:OD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:401:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:402:GLY:C | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:O | 2:B:402:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:402:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:402:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:402:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:403:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:404:PRO:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:404:PRO:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:404:PRO:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:404:PRO:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:404:PRO:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:404:PRO:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:404:PRO:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:CE | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:HZ1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:HZ2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:HZ3 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:NZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:410:LYS:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:H | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:414:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:CG2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:HG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:415:THR:OG1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:417:GLY:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:417:GLY:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:417:GLY:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:417:GLY:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:417:GLY:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:HD21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:HD22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:ND2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:418:ASN:OD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:419:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:419:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:419:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:419:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:419:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:419:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:CG | 6 | 0.24 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|-------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:420:GLU:OE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:421:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:423:ALA:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:423:ALA:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:423:ALA:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:423:ALA:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:423:ALA:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:423:ALA:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:424:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:424:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:424:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:424:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:424:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:424:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:424:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:424:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:425:LEU:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:CA | 6 | 0.24 | 0.08 | 0.22 |

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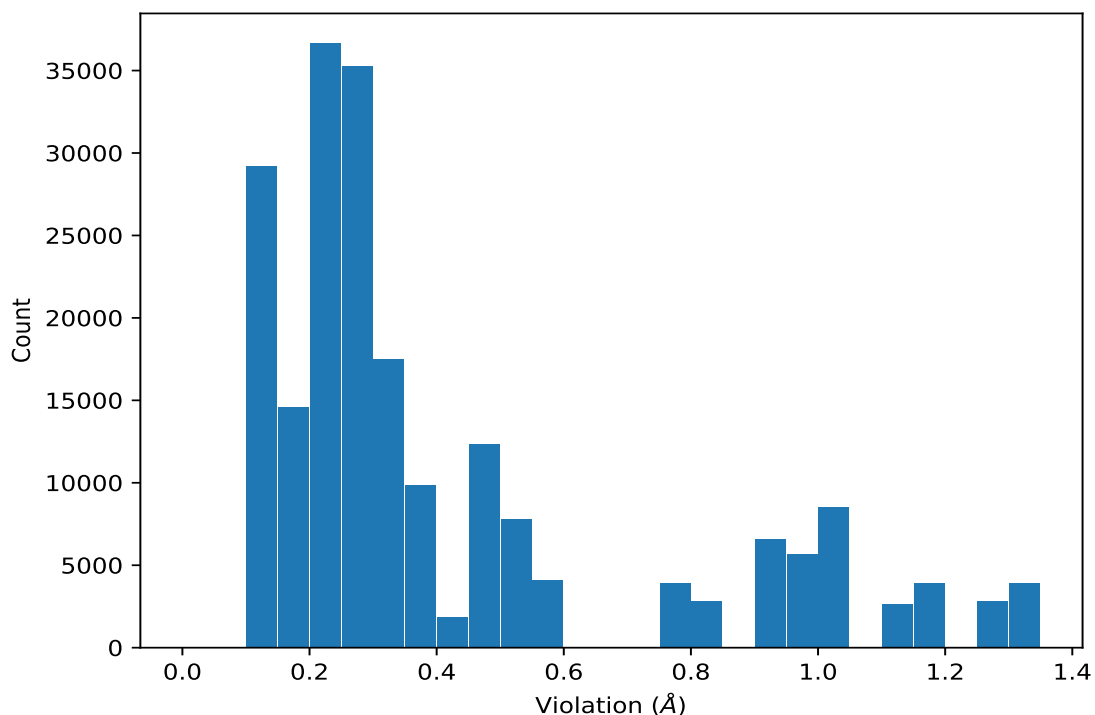
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|-------|--------------|------------------|---------------------|----------|---------------------|------------|
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:CD1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:CD2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:CE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:CE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:CZ | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:427:PHE:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:CD | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:CG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:HE21 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:HE22 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:NE2 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:428:GLN:OE1 | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:429:SER:C | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:429:SER:CA | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:429:SER:CB | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:429:SER:H | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:429:SER:HG | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:429:SER:N | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:429:SER:O | 6 | 0.24 | 0.08 | 0.22 |
| (1,2) | 1:A:8:LEU:O | 2:B:429:SER:OG | 6 | 0.24 | 0.08 | 0.22 |
| (1,6) | 1:A:47:GLY:C | 2:B:394:THR:C | 6 | 0.23 | 0.14 | 0.16 |

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 provides the 10 worst performing restraints, sorted by the violation 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) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:OG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ1 | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:SD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:OD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:OD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:H | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CB | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:OG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:HD21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:HD22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:ND2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:OD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CA | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:OE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:OG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:N | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:OG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:OG1 | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:SD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:OD1 | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:OD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ1 | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:OG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:HD21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:HD22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:ND2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:OD1 | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:OE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:OG | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:OG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:C | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:OG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:SD | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:OD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:OD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:O | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:OG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CB | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:HD21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:HD22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:ND2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:OD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:OE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:O | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:OG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:C | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:OG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:OG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:C | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:SD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:OD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:OD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:N | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:OG1 | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:HD21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:HD22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:ND2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:OD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:OE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:H | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:OG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CG | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:OG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:OG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CG | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:SD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:OD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:OD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CB | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CE | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ3 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:NZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:C | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CG2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:HG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:OG1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:HD21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:HD22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:ND2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:OD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:OE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CA | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CZ | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:OG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CD1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CD2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CZ | 9 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CD | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:HE21 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:HE22 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:NE2 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:OE1 | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:C | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:CA | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:CB | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:H | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:HG | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:N | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:O | 9 | 1.35 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:OG | 9 | 1.35 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ3 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:O | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CG | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CD | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:C | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:C | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ3 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CB | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:H | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CB | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CB | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:C | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:O | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE21 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE21 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD2 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CB | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD1 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:NZ | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE21 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:H | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CB | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CD | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CB | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:NZ | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:H | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD1 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:H | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CG | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CD | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD22 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:H | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:HG | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CG | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CB | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CA | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE2 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:H | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE1 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:C | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:C | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:O | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD2 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CG | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD2 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:C | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:ND2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:O | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CG | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:SD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CE | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CG | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ3 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:NZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CG2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:HG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:OG1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:ND2 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:OD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:N | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CZ | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CD | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE21 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE22 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:NE2 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:O | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:OE1 | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:C | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CA | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CB | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:H | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:HG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:N | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:O | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:OG | 2 | 1.32 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:N | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CG | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:H | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:O | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:O | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CZ | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:N | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CG | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:O | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE2 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE2 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ1 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:H | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:N | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:OG1 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD1 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ1 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:OD1 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:OG | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:SD | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:O | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:O | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:N | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:OG1 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:H | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CG | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CG | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CZ | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ3 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:O | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CG | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CD | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ3 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:H | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:C | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:CA | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:O | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE21 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE21 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:SD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD2 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CE | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ3 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:NZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CB | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CG2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:HG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:OG1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:ND2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:OD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD1 | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CZ | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:N | 7 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CD | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE21 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE22 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:NE2 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:OE1 | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:C | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CA | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CB | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:H | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:HG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:N | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:O | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:OG | 7 | 1.27 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:NZ | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:CA | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE21 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:H | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CB | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CD | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CB | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:NZ | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:H | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD1 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:H | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CD | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD22 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:H | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:HG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CB | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CA | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE2 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:H | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE1 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:C | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:C | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:O | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD2 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD2 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:C | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:O | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:ND2 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:O | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:C | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:H | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:O | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:O | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CZ | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CB | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CB | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:C | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:O | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE2 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE2 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ1 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:H | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CB | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:OD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CA | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:N | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:OG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:OG1 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:SD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD1 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CE | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ1 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ3 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:NZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CG2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:HG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:OG1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:ND2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:OD1 | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:OG | 4 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CZ | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CD | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE21 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE22 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:NE2 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:OE1 | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:C | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CA | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CB | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:H | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:HG | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:N | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:O | 4 | 1.18 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:OG | 4 | 1.18 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:C | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:394:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:HZ3 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:396:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:397:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:399:MET:SD | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:400:ASP:OD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:401:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:402:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:403:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:404:PRO:O | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:HZ3 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:410:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:414:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:415:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:417:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CB | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:HD21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:HD22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:ND2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:418:ASN:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:419:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:420:GLU:OE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:421:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:423:ALA:O | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:424:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:425:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:427:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:428:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:C | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:C | 2:B:429:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:394:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:HZ3 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:396:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:397:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:C | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:399:MET:SD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:400:ASP:OD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:401:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:402:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:N | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:403:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:404:PRO:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:HZ3 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:410:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:414:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:415:THR:OG1 | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:417:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:HD21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:HD22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:ND2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:418:ASN:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:419:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:420:GLU:OE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:H | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:421:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:423:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:424:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:425:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:427:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:CG | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:428:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:CA | 2:B:429:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:394:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:HZ3 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:396:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:CG | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:397:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:399:MET:SD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:400:ASP:OD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:401:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:402:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CB | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:403:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:404:PRO:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:HZ3 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:410:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:414:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:C | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:415:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:417:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:HD21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:HD22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:ND2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:418:ASN:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:419:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:420:GLU:OE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CA | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:421:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:423:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:424:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:425:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:CZ | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:427:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:428:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:H | 2:B:429:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:394:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:HZ3 | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:396:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:397:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:399:MET:SD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:400:ASP:OD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:401:LEU:O | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:402:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:403:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:404:PRO:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:HZ3 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:410:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:CG | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:414:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:415:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:417:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:HD21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:HD22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:ND2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:418:ASN:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:419:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CD | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:420:GLU:OE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:421:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:423:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:424:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:425:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:C | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:427:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:428:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:N | 2:B:429:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:394:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CA | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:HZ3 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:396:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:397:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:399:MET:SD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:400:ASP:OD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:C | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:401:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:402:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:403:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:404:PRO:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CE | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:HZ3 | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:NZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:410:LYS:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:414:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:CG2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:HG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:415:THR:OG1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:417:GLY:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:HD21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:HD22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:ND2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:418:ASN:OD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:CA | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:419:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:420:GLU:OE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:421:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:423:ALA:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:424:SER:OG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CA | 10 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:425:LEU:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CD1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CD2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:CZ | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:427:PHE:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CD | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:CG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:HE21 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:HE22 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:NE2 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:428:GLN:OE1 | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:C | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:CA | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:CB | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:H | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:HG | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:N | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:O | 10 | 1.16 |
| (1,3) | 1:A:10:GLY:O | 2:B:429:SER:OG | 10 | 1.16 |
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:CB | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:CA | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:CA | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:H | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:424:SER:CA | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:C | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:429:SER:CB | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:C | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:C | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:CB | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:404:PRO:C | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CA | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:417:GLY:CA | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CA | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:421:PHE:O | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CA | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:HE21 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CA | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:HE21 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:CD2 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:CB | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:CD1 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CB | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CB | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:NZ | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CD | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:402:GLY:CA | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CD | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:HE21 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:H | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:CB | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CD | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:CD | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:CB | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:NZ | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CG | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:419:ALA:H | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CG | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:CD1 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:CG | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:H | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:CG | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:CD | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:HD22 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:424:SER:H | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:H | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:429:SER:HG | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:H | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:H | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:CG | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:404:PRO:CB | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE21 | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:417:GLY:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE21 | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:423:ALA:CA | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE21 | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE21 | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:CE2 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:H | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:CE1 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:C | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:HE22 | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:C | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:402:GLY:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:N | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:O | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:CD2 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:N | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:CG | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:CD2 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:C | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:419:ALA:O | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:CG | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:NE2 | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:404:PRO:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:CG | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:ND2 | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:423:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:424:SER:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:O | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:O | 2:B:429:SER:O | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:O | 2:B:429:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:394:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:396:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:397:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:N | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:399:MET:SD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:400:ASP:OD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:401:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:402:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:402:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:402:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:402:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:402:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:403:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:404:PRO:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:404:PRO:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:404:PRO:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:404:PRO:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:404:PRO:CG | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:OE1 | 2:B:404:PRO:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:404:PRO:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:CE | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:HZ1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:HZ2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:HZ3 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:NZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:410:LYS:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:414:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:CG2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:HG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:415:THR:OG1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:417:GLY:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:417:GLY:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:417:GLY:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:417:GLY:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:417:GLY:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:C | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:HD21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:HD22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:ND2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:418:ASN:OD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:419:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:419:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:419:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:419:ALA:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:419:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:419:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:420:GLU:OE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:421:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:423:ALA:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:423:ALA:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:423:ALA:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:423:ALA:H | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:OE1 | 2:B:423:ALA:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:423:ALA:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:424:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:424:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:424:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:424:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:424:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:424:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:424:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:424:SER:OG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:425:LEU:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:CD1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:CD2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:CE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:CE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:CZ | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:427:PHE:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:CD | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:CG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:HE21 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:HE22 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:NE2 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:O | 7 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,8) | 1:A:49:GLN:OE1 | 2:B:428:GLN:OE1 | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:429:SER:C | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:429:SER:CA | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:429:SER:CB | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:429:SER:H | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:429:SER:HG | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:429:SER:N | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:429:SER:O | 7 | 1.13 |
| (1,8) | 1:A:49:GLN:OE1 | 2:B:429:SER:OG | 7 | 1.13 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:O | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CZ | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:N | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CG | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:C | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:O | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE2 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE2 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ1 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:H | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:N | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:OG1 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD1 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ1 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:OD1 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:OG | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:C | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:SD | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:O | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:O | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:C | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:C | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:N | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:OG1 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:H | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CG | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CG | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:C | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CZ | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ3 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:O | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CG | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CD | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:C | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:C | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ3 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:H | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:C | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:O | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE21 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE21 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD2 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD1 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:N | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:NZ | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:SD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:CA | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CE | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ3 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:NZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE21 | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CG2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:HG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:OG1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:ND2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:OD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:H | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:OG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CB | 5 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CZ | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CD | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE21 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE22 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:NE2 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:OE1 | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:C | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CA | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CB | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:H | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:HG | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:N | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:O | 5 | 1.04 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:OG | 5 | 1.04 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:CD | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:CB | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:NZ | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:C | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:419:ALA:H | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:C | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:CD1 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:C | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:H | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:CG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:CD | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:HD22 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:424:SER:H | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CA | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:429:SER:HG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CA | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CA | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:CG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:404:PRO:CB | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CB | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:417:GLY:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CB | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:423:ALA:CA | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CB | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CB | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:CE2 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:H | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:CE1 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:C | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CD | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:C | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:402:GLY:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CE | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:O | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:CD2 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CE | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:CG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:CD2 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:C | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:419:ALA:O | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:CG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:CG | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:CG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:ND2 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:424:SER:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:H | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:H | 2:B:429:SER:O | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:H | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:404:PRO:CG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:C | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:423:ALA:H | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:O | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ1 | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:O | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:CZ | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:CG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:CB | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ2 | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:CB | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:C | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:O | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:420:GLU:OE2 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:CE2 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:HZ3 | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:HZ1 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:H | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:CB | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:CA | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:N | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:N | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:N | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:394:THR:OG1 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:399:MET:SD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:OD1 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:NZ | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:404:PRO:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:HZ1 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:418:ASN:OD1 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:NZ | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:423:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:424:SER:OG | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:429:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:NZ | 2:B:429:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:C | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:394:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:396:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:397:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:399:MET:SD | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|-----------------|----------|---------------|
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:400:ASP:OD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:401:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:402:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:402:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:402:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:402:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:402:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:403:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:404:PRO:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:404:PRO:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:404:PRO:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:404:PRO:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:404:PRO:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:404:PRO:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:404:PRO:O | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:CE | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:HZ1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:HZ2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:HZ3 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:NZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:410:LYS:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:414:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:CG2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:HG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:415:THR:OG1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:417:GLY:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:417:GLY:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:417:GLY:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:417:GLY:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:417:GLY:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:CB | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:HD21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:HD22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:ND2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:418:ASN:OD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:419:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:419:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:419:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:419:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:419:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:419:ALA:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:420:GLU:OE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:421:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:423:ALA:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:423:ALA:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:423:ALA:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:423:ALA:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:423:ALA:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:423:ALA:O | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|-------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:O | 2:B:424:SER:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:424:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:424:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:424:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:424:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:424:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:424:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:424:SER:OG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:425:LEU:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:CD1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:CD2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:CE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:CE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:CZ | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:427:PHE:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:C | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:CD | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:CG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:HE21 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:HE22 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:NE2 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:428:GLN:OE1 | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:429:SER:C | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,1) | 1:A:6:LYS:O | 2:B:429:SER:CA | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:429:SER:CB | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:429:SER:H | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:429:SER:HG | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:429:SER:N | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:429:SER:O | 9 | 1.01 |
| (1,1) | 1:A:6:LYS:O | 2:B:429:SER:OG | 9 | 1.01 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:C | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:N | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:415:THR:OG1 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:H | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:CG | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:CG | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CB | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:C | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:CZ | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CA | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:HZ3 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:401:LEU:O | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:CG | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CD | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:C | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CB | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:C | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:HZ3 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CD | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CB | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:H | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:CB | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CE | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CB | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:C | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:421:PHE:O | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE21 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:CG | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE21 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CD2 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CB | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD1 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:N | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:H | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:H | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:NZ | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE21 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:H | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CB | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ1 | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CD | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CB | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:NZ | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:H | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD1 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ2 | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:H | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:CG | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CD | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:HD22 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:H | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:HG | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|----------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:HZ3 | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:CG | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CB | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:N | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CA | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:N | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:N | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:N | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CE2 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:H | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE1 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:C | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:NZ | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:394:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:396:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:C | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:397:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:399:MET:SD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:400:ASP:OD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:401:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:N | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:402:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:403:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:404:PRO:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CE | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:HZ3 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:NZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:410:LYS:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:N | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:414:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:CG2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:HG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:415:THR:OG1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:417:GLY:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:HD22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:ND2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:418:ASN:OD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:419:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:O | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|-----------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:420:GLU:OE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:421:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:423:ALA:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:424:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CD2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:425:LEU:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CD2 | 6 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|--------------|------------------|----------|---------------|
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:CZ | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:427:PHE:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CD | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:CG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE21 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:HE22 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:NE2 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:428:GLN:OE1 | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:C | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CA | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:CB | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:H | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:HG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:N | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:O | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:O | 2:B:429:SER:OG | 6 | 1.0 |
| (1,7) | 1:A:48:LYS:C | 2:B:394:THR:C | 10 | 0.99 |

10 Dihedral-angle violation analysis

No dihedral-angle restraints found