



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 07:49 AM UTC

PDB ID : 9HDI / pdb_00009hdi
BMRB ID : 50124
Title : N-terminally truncated CanA from *Pyrodicticum abyssi* - K1-CanA
Authors : Munte, C.E.; Kalbitzer, H.R.; Kreitner, R.R.; Stetter, K.O.
Deposited on : 2024-11-12

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

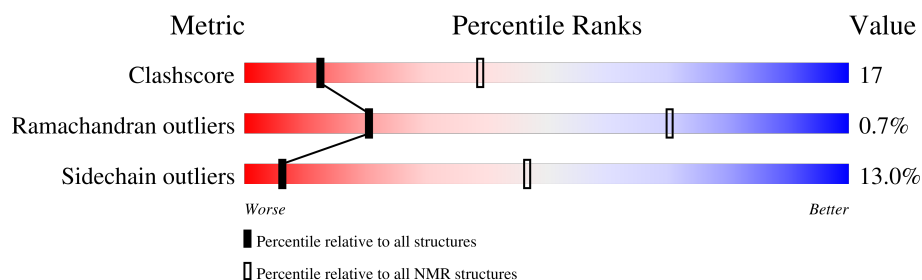
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 95%.

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 | 229148 | 14424 |
| Ramachandran outliers | 224038 | 12848 |
| Sidechain outliers | 223484 | 12823 |

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 | 183 | <div> <div></div> <div>54%</div> <div>19%</div> <div>•</div> <div>19%</div> <div>6%</div> </div> |

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:23-A:33, A:39-A:87, A:95-A:119, A:131-A:183 (138) | 0.70 | 4 |

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 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2638 atoms, of which 1317 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cannulae forming protein.

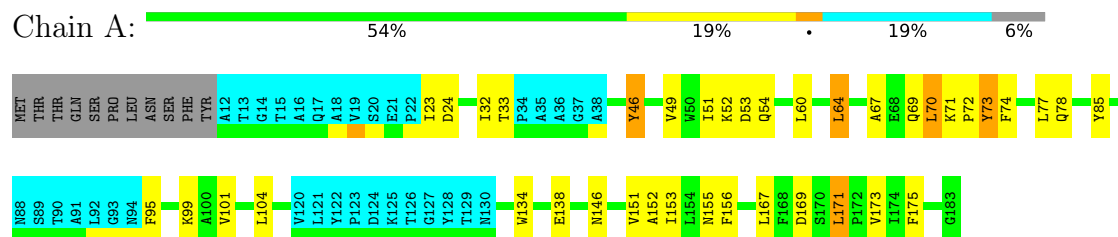
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1 | A | 172 | Total | C | H | N | O | S | 0 |
| | | | 2638 | 854 | 1317 | 205 | 261 | 1 | |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Cannulae forming protein

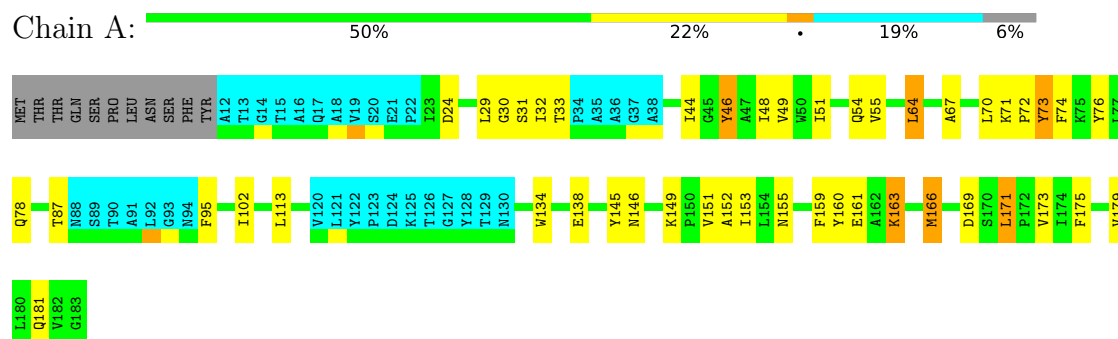


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

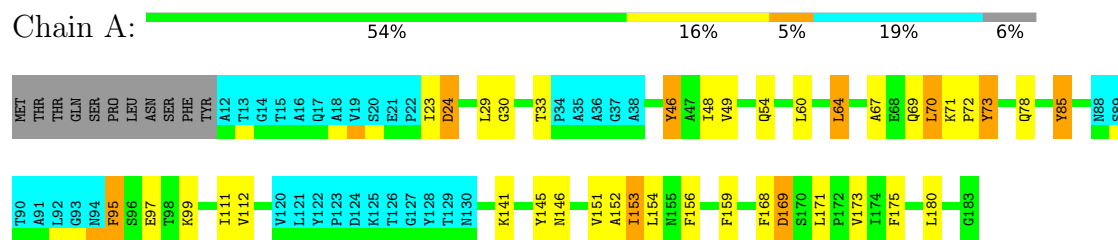
4.2.1 Score per residue for model 1

- Molecule 1: Cannulae forming protein



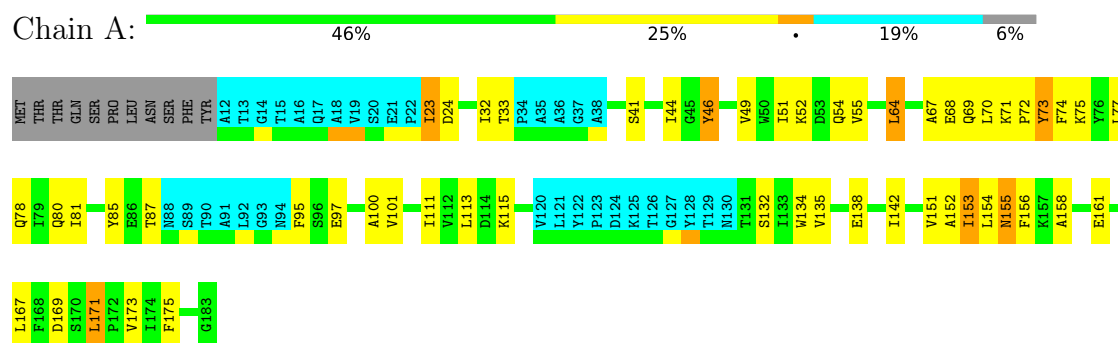
4.2.2 Score per residue for model 2

- Molecule 1: Cannulae forming protein



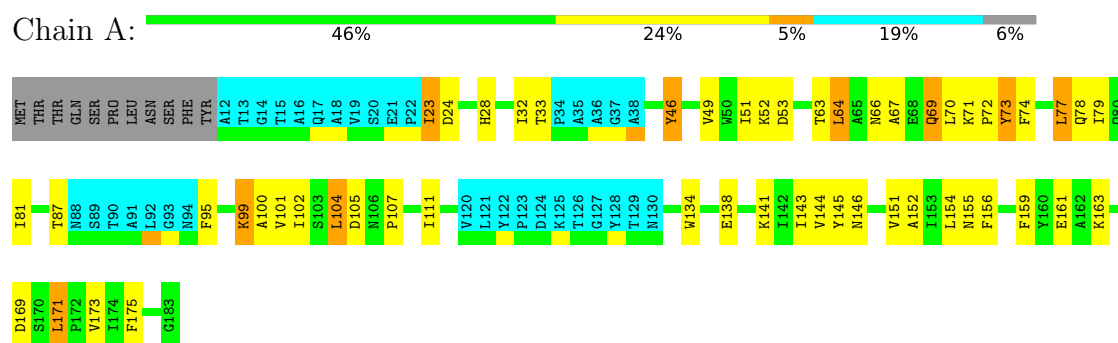
4.2.3 Score per residue for model 3

- Molecule 1: Cannulae forming protein



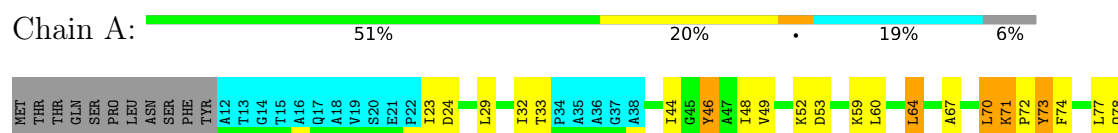
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Cannulae forming protein



4.2.5 Score per residue for model 5

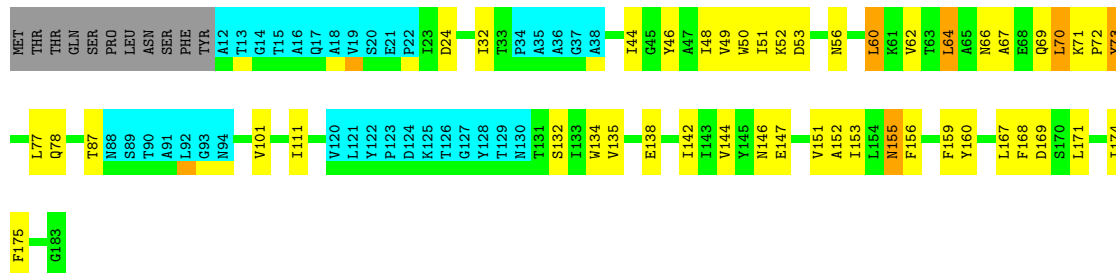
- Molecule 1: Cannulae forming protein





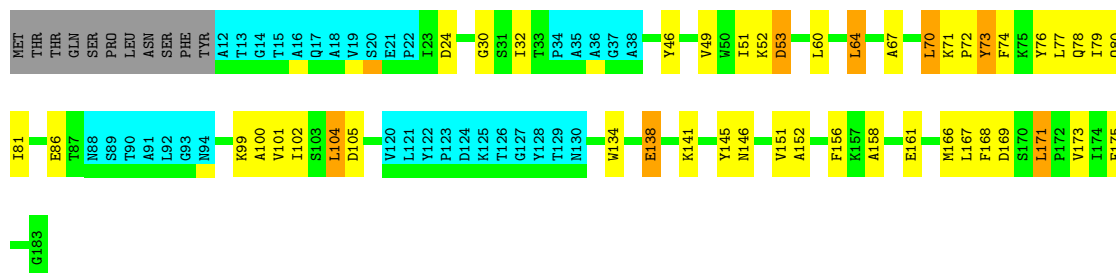
4.2.6 Score per residue for model 6

- Molecule 1: Cannulae forming protein



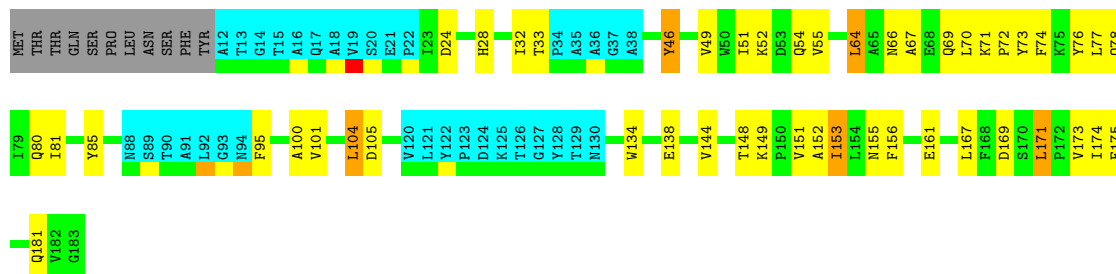
4.2.7 Score per residue for model 7

- Molecule 1: Cannulae forming protein



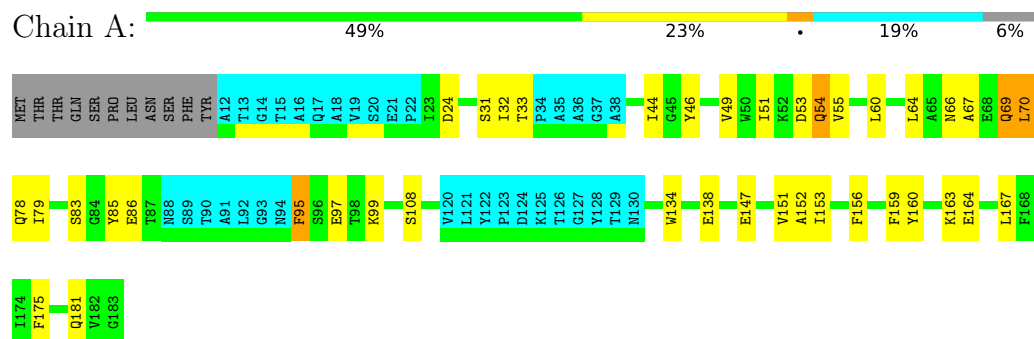
4.2.8 Score per residue for model 8

- Molecule 1: Cannulae forming protein



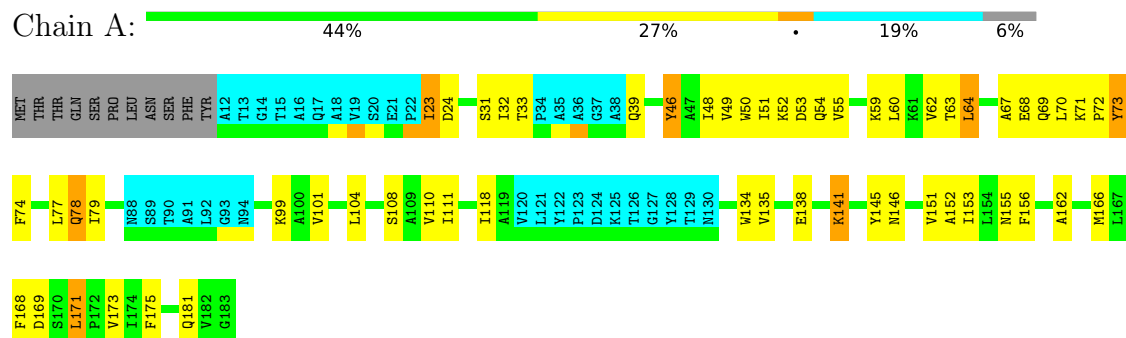
4.2.9 Score per residue for model 9

- Molecule 1: Cannulae forming protein



4.2.10 Score per residue for model 10

- Molecule 1: Cannulae forming protein



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| CNS | structure calculation | |
| CNS | refinement | |

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 | 2170 |
| Number of shifts mapped to atoms | 2170 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 95% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.50±0.01 | 0±0/1112 (0.0± 0.0%) | 0.80±0.01 | 0±0/1515 (0.0± 0.0%) |
| All | All | 0.50 | 1/11120 (0.0%) | 0.80 | 0/15150 (0.0%) |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 138 | GLU | N-CA | -5.53 | 1.41 | 1.46 | 7 | 1 |

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 | 1089 | 1097 | 1096 | 37±7 |
| All | All | 10890 | 10970 | 10960 | 366 |

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 17.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:64:LEU:HD23 | 1:A:67:ALA:HB2 | 1.04 | 1.22 | 2 | 10 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:135:VAL:HG22 | 1:A:153:ILE:HG21 | 0.83 | 1.51 | 10 | 3 |
| 1:A:64:LEU:HD23 | 1:A:67:ALA:CB | 0.80 | 2.06 | 2 | 10 |
| 1:A:51:ILE:HG23 | 1:A:55:VAL:HG13 | 0.80 | 1.53 | 9 | 5 |
| 1:A:163:LYS:O | 1:A:166:MET:HE2 | 0.78 | 1.78 | 1 | 1 |
| 1:A:70:LEU:HD22 | 1:A:171:LEU:CD1 | 0.75 | 2.11 | 4 | 2 |
| 1:A:51:ILE:CG2 | 1:A:55:VAL:HG13 | 0.72 | 2.14 | 9 | 3 |
| 1:A:143:ILE:HG22 | 1:A:144:VAL:HG23 | 0.71 | 1.62 | 5 | 2 |
| 1:A:30:GLY:O | 1:A:173:VAL:HG12 | 0.70 | 1.86 | 1 | 3 |
| 1:A:85:TYR:CE1 | 1:A:153:ILE:HD13 | 0.70 | 2.21 | 3 | 3 |
| 1:A:85:TYR:CD1 | 1:A:153:ILE:HD13 | 0.69 | 2.22 | 2 | 1 |
| 1:A:166:MET:HE1 | 1:A:168:PHE:CE2 | 0.69 | 2.23 | 10 | 1 |
| 1:A:49:VAL:HB | 1:A:152:ALA:HB3 | 0.68 | 1.65 | 10 | 9 |
| 1:A:77:LEU:HD22 | 1:A:78:GLN:N | 0.67 | 2.05 | 4 | 2 |
| 1:A:104:LEU:HD12 | 1:A:105:ASP:N | 0.67 | 2.05 | 4 | 3 |
| 1:A:29:LEU:HD13 | 1:A:173:VAL:O | 0.67 | 1.89 | 1 | 3 |
| 1:A:73:TYR:OH | 1:A:171:LEU:HD11 | 0.65 | 1.92 | 10 | 1 |
| 1:A:32:ILE:HG21 | 1:A:74:PHE:CZ | 0.64 | 2.27 | 5 | 8 |
| 1:A:85:TYR:CZ | 1:A:153:ILE:HD13 | 0.64 | 2.27 | 3 | 2 |
| 1:A:153:ILE:HD12 | 1:A:153:ILE:N | 0.64 | 2.08 | 2 | 3 |
| 1:A:70:LEU:HD22 | 1:A:171:LEU:HD11 | 0.63 | 1.71 | 4 | 2 |
| 1:A:180:LEU:HD22 | 1:A:181:GLN:N | 0.63 | 2.07 | 5 | 1 |
| 1:A:64:LEU:CD2 | 1:A:67:ALA:HB2 | 0.62 | 2.19 | 4 | 5 |
| 1:A:73:TYR:CE1 | 1:A:74:PHE:CE2 | 0.62 | 2.88 | 8 | 1 |
| 1:A:166:MET:O | 1:A:166:MET:HE3 | 0.61 | 1.95 | 1 | 1 |
| 1:A:69:GLN:NE2 | 1:A:70:LEU:HD23 | 0.61 | 2.11 | 4 | 1 |
| 1:A:49:VAL:O | 1:A:151:VAL:HG23 | 0.61 | 1.95 | 3 | 8 |
| 1:A:63:THR:HG23 | 1:A:107:PRO:O | 0.60 | 1.96 | 4 | 1 |
| 1:A:99:LYS:CE | 1:A:154:LEU:HD22 | 0.60 | 2.26 | 4 | 1 |
| 1:A:100:ALA:HB3 | 1:A:111:ILE:CD1 | 0.59 | 2.28 | 3 | 2 |
| 1:A:64:LEU:HD11 | 1:A:173:VAL:CG2 | 0.59 | 2.28 | 4 | 5 |
| 1:A:64:LEU:HD12 | 1:A:175:PHE:CE2 | 0.58 | 2.33 | 8 | 5 |
| 1:A:64:LEU:HD23 | 1:A:67:ALA:CA | 0.58 | 2.28 | 8 | 6 |
| 1:A:70:LEU:HD23 | 1:A:171:LEU:CD1 | 0.58 | 2.28 | 5 | 1 |
| 1:A:152:ALA:C | 1:A:153:ILE:HD12 | 0.58 | 2.23 | 3 | 2 |
| 1:A:64:LEU:HD12 | 1:A:175:PHE:CE1 | 0.58 | 2.34 | 9 | 4 |
| 1:A:23:ILE:HD12 | 1:A:23:ILE:N | 0.57 | 2.15 | 4 | 2 |
| 1:A:44:ILE:HD11 | 1:A:156:PHE:HB3 | 0.57 | 1.76 | 9 | 2 |
| 1:A:73:TYR:O | 1:A:166:MET:HE2 | 0.57 | 1.99 | 10 | 1 |
| 1:A:74:PHE:CE2 | 1:A:171:LEU:HD23 | 0.57 | 2.35 | 1 | 1 |
| 1:A:51:ILE:HG22 | 1:A:53:ASP:O | 0.57 | 1.99 | 4 | 3 |
| 1:A:73:TYR:CE2 | 1:A:171:LEU:HD11 | 0.57 | 2.35 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:154:LEU:N | 1:A:154:LEU:HD12 | 0.56 | 2.14 | 2 | 1 |
| 1:A:51:ILE:HD12 | 1:A:55:VAL:HG11 | 0.56 | 1.76 | 8 | 1 |
| 1:A:99:LYS:HE3 | 1:A:154:LEU:HD22 | 0.55 | 1.78 | 4 | 1 |
| 1:A:79:ILE:O | 1:A:101:VAL:HG23 | 0.54 | 2.03 | 4 | 1 |
| 1:A:49:VAL:C | 1:A:151:VAL:HG23 | 0.54 | 2.27 | 5 | 8 |
| 1:A:80:GLN:HG3 | 1:A:101:VAL:HG22 | 0.54 | 1.79 | 3 | 3 |
| 1:A:77:LEU:C | 1:A:77:LEU:HD13 | 0.54 | 2.27 | 4 | 2 |
| 1:A:48:ILE:HG21 | 1:A:50:TRP:CZ2 | 0.54 | 2.38 | 6 | 2 |
| 1:A:73:TYR:CZ | 1:A:171:LEU:HD11 | 0.54 | 2.38 | 9 | 2 |
| 1:A:73:TYR:N | 1:A:73:TYR:CD1 | 0.54 | 2.76 | 10 | 1 |
| 1:A:51:ILE:HG23 | 1:A:55:VAL:CG1 | 0.53 | 2.31 | 9 | 2 |
| 1:A:48:ILE:HD13 | 1:A:153:ILE:HD12 | 0.53 | 1.79 | 5 | 1 |
| 1:A:77:LEU:HD23 | 1:A:78:GLN:N | 0.53 | 2.19 | 3 | 5 |
| 1:A:70:LEU:O | 1:A:73:TYR:CE2 | 0.53 | 2.62 | 3 | 5 |
| 1:A:51:ILE:CD1 | 1:A:118:ILE:HD12 | 0.53 | 2.34 | 10 | 1 |
| 1:A:73:TYR:CE1 | 1:A:74:PHE:CZ | 0.52 | 2.97 | 8 | 1 |
| 1:A:70:LEU:O | 1:A:73:TYR:CE1 | 0.52 | 2.63 | 5 | 5 |
| 1:A:44:ILE:C | 1:A:44:ILE:HD12 | 0.52 | 2.30 | 3 | 1 |
| 1:A:132:SER:OG | 1:A:142:ILE:HG23 | 0.52 | 2.04 | 3 | 2 |
| 1:A:73:TYR:OH | 1:A:171:LEU:CD2 | 0.51 | 2.58 | 8 | 1 |
| 1:A:44:ILE:HD11 | 1:A:156:PHE:CB | 0.51 | 2.36 | 3 | 1 |
| 1:A:73:TYR:CE2 | 1:A:74:PHE:CE1 | 0.51 | 2.99 | 10 | 1 |
| 1:A:69:GLN:HE21 | 1:A:70:LEU:HD23 | 0.51 | 1.64 | 4 | 2 |
| 1:A:63:THR:HG23 | 1:A:108:SER:HB3 | 0.50 | 1.82 | 10 | 1 |
| 1:A:73:TYR:CZ | 1:A:74:PHE:CZ | 0.50 | 3.00 | 8 | 1 |
| 1:A:81:ILE:HD12 | 1:A:100:ALA:O | 0.50 | 2.06 | 7 | 4 |
| 1:A:156:PHE:N | 1:A:156:PHE:CD1 | 0.49 | 2.79 | 7 | 6 |
| 1:A:156:PHE:CD2 | 1:A:156:PHE:N | 0.49 | 2.80 | 9 | 3 |
| 1:A:70:LEU:HA | 1:A:73:TYR:OH | 0.49 | 2.07 | 10 | 1 |
| 1:A:167:LEU:C | 1:A:167:LEU:HD23 | 0.49 | 2.33 | 3 | 4 |
| 1:A:180:LEU:C | 1:A:180:LEU:HD23 | 0.49 | 2.32 | 2 | 1 |
| 1:A:64:LEU:CD1 | 1:A:175:PHE:CZ | 0.48 | 2.96 | 8 | 9 |
| 1:A:153:ILE:N | 1:A:153:ILE:CD1 | 0.48 | 2.76 | 3 | 2 |
| 1:A:167:LEU:C | 1:A:167:LEU:HD13 | 0.48 | 2.33 | 8 | 1 |
| 1:A:59:LYS:CE | 1:A:110:VAL:HG13 | 0.48 | 2.38 | 10 | 1 |
| 1:A:73:TYR:CE2 | 1:A:171:LEU:CD1 | 0.48 | 2.97 | 8 | 1 |
| 1:A:32:ILE:HG23 | 1:A:160:TYR:CZ | 0.47 | 2.44 | 6 | 3 |
| 1:A:143:ILE:HD13 | 1:A:153:ILE:HG13 | 0.47 | 1.85 | 5 | 1 |
| 1:A:32:ILE:HG21 | 1:A:74:PHE:HZ | 0.47 | 1.68 | 8 | 1 |
| 1:A:73:TYR:OH | 1:A:74:PHE:CZ | 0.47 | 2.67 | 8 | 1 |
| 1:A:64:LEU:CD1 | 1:A:175:PHE:CE2 | 0.47 | 2.98 | 1 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:73:TYR:OH | 1:A:171:LEU:CD1 | 0.47 | 2.61 | 10 | 3 |
| 1:A:113:LEU:HD21 | 1:A:154:LEU:HD21 | 0.47 | 1.86 | 3 | 2 |
| 1:A:180:LEU:HD22 | 1:A:180:LEU:C | 0.47 | 2.34 | 5 | 1 |
| 1:A:100:ALA:HB3 | 1:A:111:ILE:HD13 | 0.46 | 1.87 | 3 | 1 |
| 1:A:144:VAL:HG11 | 1:A:148:THR:OG1 | 0.46 | 2.11 | 8 | 1 |
| 1:A:79:ILE:C | 1:A:101:VAL:HG23 | 0.46 | 2.36 | 5 | 1 |
| 1:A:62:VAL:CG1 | 1:A:175:PHE:CD2 | 0.46 | 2.99 | 6 | 1 |
| 1:A:85:TYR:CE1 | 1:A:153:ILE:CG1 | 0.46 | 2.99 | 9 | 1 |
| 1:A:46:TYR:CD1 | 1:A:46:TYR:N | 0.46 | 2.83 | 1 | 3 |
| 1:A:85:TYR:OH | 1:A:153:ILE:HD13 | 0.46 | 2.10 | 3 | 1 |
| 1:A:71:LYS:N | 1:A:72:PRO:CD | 0.46 | 2.79 | 7 | 8 |
| 1:A:74:PHE:CZ | 1:A:171:LEU:HD23 | 0.46 | 2.46 | 1 | 1 |
| 1:A:64:LEU:HD21 | 1:A:70:LEU:HD12 | 0.46 | 1.88 | 8 | 1 |
| 1:A:64:LEU:CD1 | 1:A:175:PHE:CE1 | 0.45 | 2.99 | 2 | 5 |
| 1:A:46:TYR:N | 1:A:46:TYR:CD2 | 0.45 | 2.85 | 3 | 2 |
| 1:A:95:PHE:CE2 | 1:A:97:GLU:CG | 0.45 | 2.99 | 3 | 1 |
| 1:A:79:ILE:HD13 | 1:A:175:PHE:HZ | 0.45 | 1.71 | 10 | 1 |
| 1:A:95:PHE:CD2 | 1:A:95:PHE:O | 0.45 | 2.69 | 9 | 3 |
| 1:A:145:TYR:CE2 | 1:A:146:ASN:ND2 | 0.45 | 2.85 | 2 | 1 |
| 1:A:78:GLN:O | 1:A:159:PHE:N | 0.45 | 2.47 | 6 | 4 |
| 1:A:173:VAL:HG21 | 1:A:175:PHE:CE2 | 0.45 | 2.47 | 9 | 1 |
| 1:A:48:ILE:HG12 | 1:A:153:ILE:HD12 | 0.45 | 1.88 | 1 | 1 |
| 1:A:101:VAL:O | 1:A:101:VAL:HG23 | 0.45 | 2.12 | 10 | 2 |
| 1:A:44:ILE:HG21 | 1:A:158:ALA:HB2 | 0.45 | 1.88 | 5 | 2 |
| 1:A:69:GLN:NE2 | 1:A:70:LEU:CD1 | 0.45 | 2.79 | 9 | 1 |
| 1:A:134:TRP:CD1 | 1:A:138:GLU:O | 0.45 | 2.70 | 7 | 8 |
| 1:A:48:ILE:CD1 | 1:A:153:ILE:HD12 | 0.45 | 2.41 | 5 | 1 |
| 1:A:151:VAL:HG12 | 1:A:152:ALA:N | 0.45 | 2.27 | 10 | 2 |
| 1:A:76:TYR:CE2 | 1:A:161:GLU:CB | 0.45 | 3.00 | 8 | 1 |
| 1:A:167:LEU:HD13 | 1:A:168:PHE:N | 0.45 | 2.25 | 7 | 1 |
| 1:A:66:ASN:ND2 | 1:A:172:PRO:O | 0.45 | 2.50 | 9 | 1 |
| 1:A:180:LEU:H | 1:A:180:LEU:HD13 | 0.45 | 1.71 | 5 | 1 |
| 1:A:167:LEU:HD13 | 1:A:167:LEU:C | 0.44 | 2.37 | 7 | 1 |
| 1:A:145:TYR:CD1 | 1:A:146:ASN:N | 0.44 | 2.85 | 10 | 1 |
| 1:A:81:ILE:HG22 | 1:A:99:LYS:NZ | 0.44 | 2.27 | 4 | 1 |
| 1:A:99:LYS:HD2 | 1:A:111:ILE:HG23 | 0.44 | 1.90 | 2 | 1 |
| 1:A:112:VAL:HG13 | 1:A:112:VAL:O | 0.44 | 2.13 | 2 | 1 |
| 1:A:70:LEU:HD23 | 1:A:73:TYR:OH | 0.44 | 2.13 | 10 | 1 |
| 1:A:74:PHE:CE1 | 1:A:171:LEU:HD23 | 0.44 | 2.47 | 9 | 1 |
| 1:A:71:LYS:N | 1:A:72:PRO:HD2 | 0.43 | 2.28 | 8 | 2 |
| 1:A:44:ILE:HD11 | 1:A:79:ILE:HG23 | 0.43 | 1.89 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:59:LYS:HE2 | 1:A:110:VAL:HG13 | 0.43 | 1.90 | 10 | 1 |
| 1:A:70:LEU:HD22 | 1:A:171:LEU:HD21 | 0.43 | 1.90 | 8 | 1 |
| 1:A:69:GLN:NE2 | 1:A:70:LEU:HD12 | 0.43 | 2.28 | 9 | 1 |
| 1:A:113:LEU:HD23 | 1:A:152:ALA:HB1 | 0.43 | 1.90 | 1 | 1 |
| 1:A:76:TYR:CE1 | 1:A:161:GLU:CB | 0.43 | 3.01 | 7 | 1 |
| 1:A:70:LEU:HD23 | 1:A:171:LEU:HD11 | 0.43 | 1.90 | 10 | 1 |
| 1:A:151:VAL:CG1 | 1:A:152:ALA:N | 0.43 | 2.82 | 6 | 2 |
| 1:A:28:HIS:CB | 1:A:46:TYR:CD2 | 0.43 | 3.02 | 4 | 2 |
| 1:A:66:ASN:OD1 | 1:A:69:GLN:HB3 | 0.42 | 2.13 | 4 | 1 |
| 1:A:71:LYS:HG2 | 1:A:104:LEU:HD22 | 0.42 | 1.91 | 10 | 1 |
| 1:A:70:LEU:HD13 | 1:A:77:LEU:CD1 | 0.42 | 2.44 | 7 | 1 |
| 1:A:66:ASN:CB | 1:A:174:ILE:HB | 0.42 | 2.44 | 8 | 1 |
| 1:A:155:ASN:C | 1:A:156:PHE:CD1 | 0.42 | 2.98 | 6 | 3 |
| 1:A:62:VAL:HG12 | 1:A:175:PHE:CD2 | 0.42 | 2.49 | 6 | 1 |
| 1:A:64:LEU:HD12 | 1:A:175:PHE:CD2 | 0.42 | 2.48 | 8 | 1 |
| 1:A:73:TYR:OH | 1:A:171:LEU:HD21 | 0.42 | 2.14 | 8 | 1 |
| 1:A:79:ILE:HG21 | 1:A:175:PHE:CZ | 0.42 | 2.50 | 10 | 1 |
| 1:A:66:ASN:HB2 | 1:A:174:ILE:HB | 0.42 | 1.91 | 8 | 2 |
| 1:A:151:VAL:HG11 | 1:A:153:ILE:HD11 | 0.42 | 1.92 | 6 | 1 |
| 1:A:95:PHE:C | 1:A:95:PHE:CD1 | 0.42 | 2.97 | 8 | 1 |
| 1:A:60:LEU:CD2 | 1:A:111:ILE:HD11 | 0.42 | 2.45 | 6 | 1 |
| 1:A:53:ASP:O | 1:A:54:GLN:O | 0.42 | 2.38 | 9 | 1 |
| 1:A:73:TYR:HH | 1:A:171:LEU:HD11 | 0.42 | 1.72 | 10 | 1 |
| 1:A:95:PHE:CD2 | 1:A:95:PHE:C | 0.41 | 2.98 | 2 | 3 |
| 1:A:74:PHE:CE2 | 1:A:171:LEU:CD2 | 0.41 | 3.03 | 1 | 1 |
| 1:A:44:ILE:CG2 | 1:A:158:ALA:HB2 | 0.41 | 2.45 | 3 | 1 |
| 1:A:145:TYR:CD1 | 1:A:146:ASN:OD1 | 0.41 | 2.74 | 4 | 1 |
| 1:A:166:MET:CE | 1:A:168:PHE:CE2 | 0.41 | 2.99 | 10 | 1 |
| 1:A:48:ILE:CG2 | 1:A:151:VAL:HG21 | 0.41 | 2.45 | 2 | 2 |
| 1:A:145:TYR:CE2 | 1:A:146:ASN:OD1 | 0.41 | 2.74 | 1 | 1 |
| 1:A:179:VAL:O | 1:A:179:VAL:HG13 | 0.41 | 2.16 | 1 | 1 |
| 1:A:78:GLN:O | 1:A:158:ALA:HA | 0.41 | 2.16 | 7 | 2 |
| 1:A:70:LEU:O | 1:A:73:TYR:CD2 | 0.41 | 2.74 | 3 | 1 |
| 1:A:144:VAL:CG1 | 1:A:147:GLU:CG | 0.41 | 2.99 | 6 | 1 |
| 1:A:162:ALA:HB1 | 1:A:166:MET:CE | 0.41 | 2.46 | 10 | 1 |
| 1:A:48:ILE:CG2 | 1:A:151:VAL:CG2 | 0.41 | 2.99 | 2 | 1 |
| 1:A:95:PHE:O | 1:A:95:PHE:CD2 | 0.41 | 2.74 | 4 | 1 |
| 1:A:60:LEU:C | 1:A:60:LEU:HD12 | 0.41 | 2.41 | 5 | 1 |
| 1:A:95:PHE:CD1 | 1:A:95:PHE:O | 0.41 | 2.74 | 1 | 2 |
| 1:A:70:LEU:HD11 | 1:A:171:LEU:HB3 | 0.41 | 1.92 | 9 | 1 |
| 1:A:62:VAL:CG2 | 1:A:111:ILE:CD1 | 0.41 | 2.99 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:95:PHE:CD1 | 1:A:95:PHE:C | 0.40 | 2.99 | 1 | 1 |
| 1:A:23:ILE:HG22 | 1:A:24:ASP:N | 0.40 | 2.30 | 2 | 1 |
| 1:A:95:PHE:CD1 | 1:A:97:GLU:OE2 | 0.40 | 2.74 | 2 | 1 |
| 1:A:70:LEU:CD1 | 1:A:77:LEU:CD1 | 0.40 | 2.99 | 7 | 1 |
| 1:A:46:TYR:CE2 | 1:A:141:LYS:HD3 | 0.40 | 2.52 | 10 | 1 |
| 1:A:70:LEU:HA | 1:A:73:TYR:CE1 | 0.40 | 2.51 | 1 | 1 |
| 1:A:166:MET:O | 1:A:166:MET:CE | 0.40 | 2.66 | 1 | 1 |
| 1:A:167:LEU:HD23 | 1:A:168:PHE:N | 0.40 | 2.31 | 6 | 1 |
| 1:A:145:TYR:CE2 | 1:A:146:ASN:CG | 0.40 | 3.00 | 7 | 1 |
| 1:A:76:TYR:CE2 | 1:A:161:GLU:CD | 0.40 | 3.00 | 1 | 1 |
| 1:A:78:GLN:CB | 1:A:159:PHE:HB2 | 0.40 | 2.46 | 4 | 1 |
| 1:A:70:LEU:CD2 | 1:A:171:LEU:CD1 | 0.40 | 3.00 | 5 | 1 |
| 1:A:79:ILE:O | 1:A:102:ILE:N | 0.40 | 2.54 | 7 | 1 |
| 1:A:64:LEU:HD23 | 1:A:67:ALA:HA | 0.40 | 1.92 | 8 | 1 |

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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 | 137/183 (75%) | 134±1 (97±1%) | 2±1 (2±1%) | 1±1 (1±0%) | 20 | 70 |
| All | All | 1370/1830 (75%) | 1335 (97%) | 25 (2%) | 10 (1%) | 20 | 70 |

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 54 | GLN | 6 |
| 1 | A | 169 | ASP | 1 |
| 1 | A | 53 | ASP | 1 |
| 1 | A | 146 | ASN | 1 |
| 1 | A | 39 | GLN | 1 |

6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|---------------|--------------|-------------|----|
| 1 | A | 122/156 (78%) | 106±2 (87±2%) | 16±2 (13±2%) | 6 | 47 |
| All | All | 1220/1560 (78%) | 1061 (87%) | 159 (13%) | 6 | 47 |

All 45 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 24 | ASP | 10 |
| 1 | A | 46 | TYR | 10 |
| 1 | A | 169 | ASP | 10 |
| 1 | A | 171 | LEU | 10 |
| 1 | A | 64 | LEU | 9 |
| 1 | A | 73 | TYR | 9 |
| 1 | A | 33 | THR | 8 |
| 1 | A | 155 | ASN | 7 |
| 1 | A | 52 | LYS | 7 |
| 1 | A | 69 | GLN | 6 |
| 1 | A | 60 | LEU | 5 |
| 1 | A | 70 | LEU | 5 |
| 1 | A | 181 | GLN | 4 |
| 1 | A | 141 | LYS | 4 |
| 1 | A | 23 | ILE | 4 |
| 1 | A | 99 | LYS | 4 |
| 1 | A | 31 | SER | 3 |
| 1 | A | 163 | LYS | 3 |
| 1 | A | 166 | MET | 3 |
| 1 | A | 153 | ILE | 3 |
| 1 | A | 104 | LEU | 3 |
| 1 | A | 102 | ILE | 2 |
| 1 | A | 149 | LYS | 2 |
| 1 | A | 85 | TYR | 2 |
| 1 | A | 95 | PHE | 2 |
| 1 | A | 68 | GLU | 2 |
| 1 | A | 161 | GLU | 2 |
| 1 | A | 53 | ASP | 2 |
| 1 | A | 86 | GLU | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 44 | ILE | 1 |
| 1 | A | 168 | PHE | 1 |
| 1 | A | 41 | SER | 1 |
| 1 | A | 75 | LYS | 1 |
| 1 | A | 115 | LYS | 1 |
| 1 | A | 77 | LEU | 1 |
| 1 | A | 59 | LYS | 1 |
| 1 | A | 71 | LYS | 1 |
| 1 | A | 180 | LEU | 1 |
| 1 | A | 56 | ASN | 1 |
| 1 | A | 83 | SER | 1 |
| 1 | A | 97 | GLU | 1 |
| 1 | A | 108 | SER | 1 |
| 1 | A | 147 | GLU | 1 |
| 1 | A | 164 | GLU | 1 |
| 1 | A | 78 | GLN | 1 |

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 95% for the well-defined parts and 95% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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 | 2170 |
| Number of shifts mapped to atoms | 2170 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 3 |

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 172 | 0.11 ± 0.14 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 161 | -0.06 ± 0.14 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 154 | 0.43 ± 0.13 | None needed (< 0.5 ppm) |
| ^{15}N | 169 | 0.32 ± 0.24 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 95%, i.e. 1806 atoms were assigned a chemical shift out of a possible 1894. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone | 677/685 (99%) | 277/277 (100%) | 268/276 (97%) | 132/132 (100%) |
| Sidechain | 989/1053 (94%) | 675/690 (98%) | 302/339 (89%) | 12/24 (50%) |

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| | Total | ¹H | ¹³C | ¹⁵N |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 140/156 (90%) | 73/75 (97%) | 65/77 (84%) | 2/4 (50%) |
| Overall | 1806/1894 (95%) | 1025/1042 (98%) | 635/692 (92%) | 146/160 (91%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 95%, i.e. 2162 atoms were assigned a chemical shift out of a possible 2278. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone | 827/853 (97%) | 339/346 (98%) | 326/344 (95%) | 162/163 (99%) |
| Sidechain | 1179/1251 (94%) | 806/821 (98%) | 357/401 (89%) | 16/29 (55%) |
| Aromatic | 156/174 (90%) | 81/83 (98%) | 73/87 (84%) | 2/4 (50%) |
| Overall | 2162/2278 (95%) | 1226/1250 (98%) | 756/832 (91%) | 180/196 (92%) |

7.1.4 Statistically unusual chemical shifts ⓘ

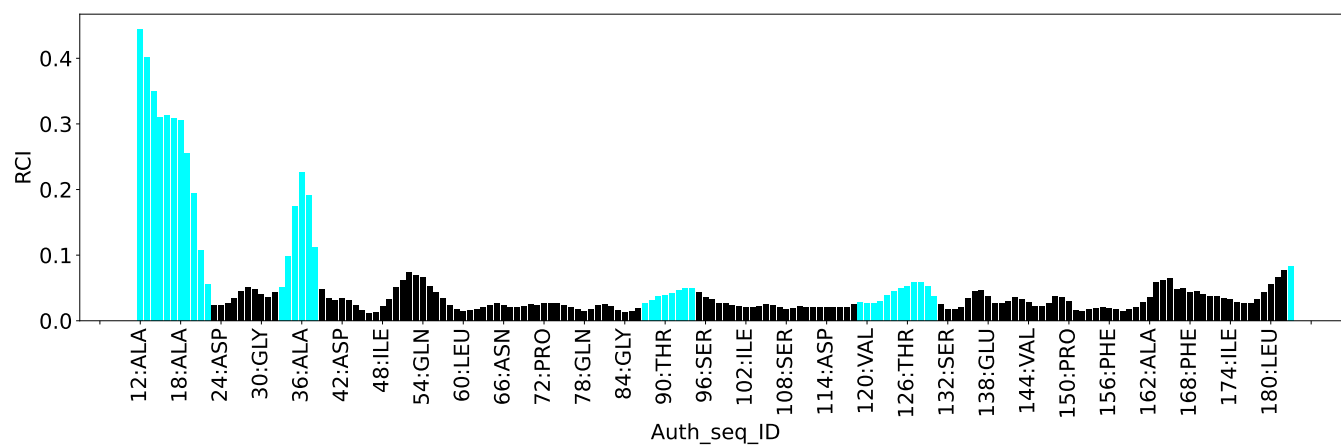
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 87 | THR | HG1 | 5.41 | 0.08 – 2.19 | 20.2 |
| 1 | A | 86 | GLU | HB2 | 0.59 | 1.00 – 3.05 | -7.0 |
| 1 | A | 146 | ASN | HB3 | 1.09 | 1.12 – 4.38 | -5.1 |

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 3318 |
| Intra-residue ($ i-j =0$) | 914 |
| Sequential ($ i-j =1$) | 736 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 394 |
| Long range ($ i-j \geq 5$) | 1220 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 54 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 284 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 19.7 |
| Number of long range restraints per residue ¹ | 7.0 |

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) | 98.3 | 0.2 |
| 0.2-0.5 (Medium) | 124.9 | 0.5 |
| >0.5 (Large) | 57.4 | 1.18 |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 67.0 | 9.99 |
| 10.0-20.0 (Medium) | 1.0 | 17.55 |
| >20.0 (Large) | 4.1 | 43.26 |

9 Distance violation analysis ⓘ

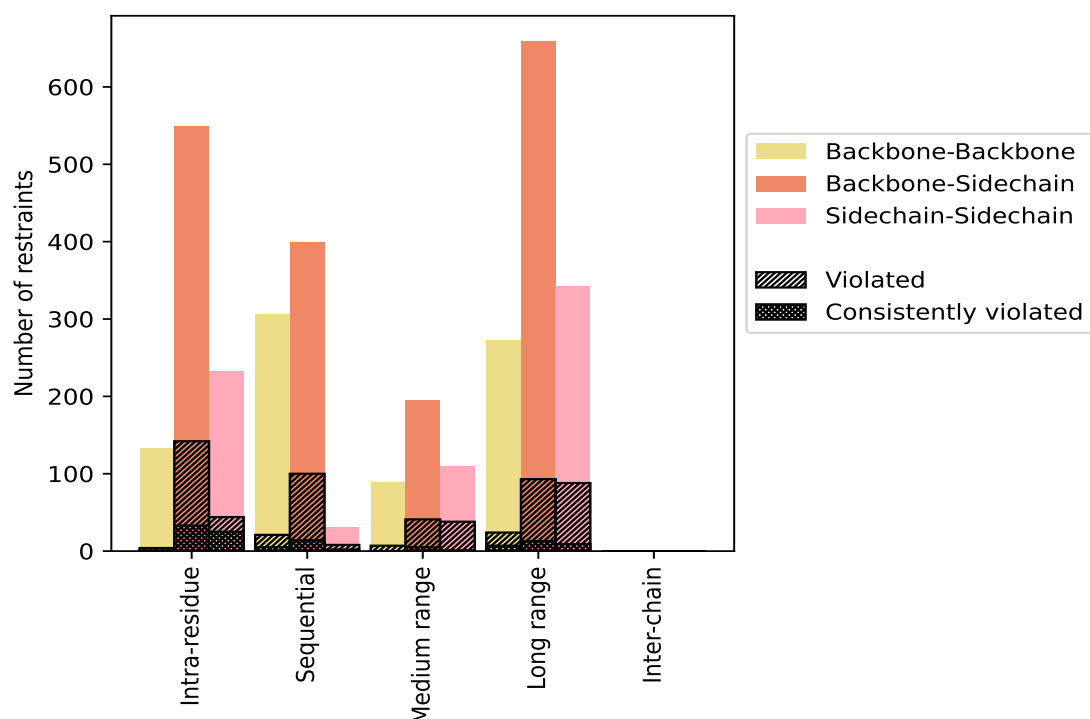
9.1 Summary of distance violations ⓘ

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 ($i-j =0$) | 914 | 27.5 | 190 | 20.8 | 5.7 | 59 | 6.5 | 1.8 |
| Backbone-Backbone | 133 | 4.0 | 4 | 3.0 | 0.1 | 1 | 0.8 | 0.0 |
| Backbone-Sidechain | 549 | 16.5 | 142 | 25.9 | 4.3 | 33 | 6.0 | 1.0 |
| Sidechain-Sidechain | 232 | 7.0 | 44 | 19.0 | 1.3 | 25 | 10.8 | 0.8 |
| Sequential ($i-j =1$) | 736 | 22.2 | 129 | 17.5 | 3.9 | 21 | 2.9 | 0.6 |
| Backbone-Backbone | 306 | 9.2 | 21 | 6.9 | 0.6 | 5 | 1.6 | 0.2 |
| Backbone-Sidechain | 399 | 12.0 | 100 | 25.1 | 3.0 | 14 | 3.5 | 0.4 |
| Sidechain-Sidechain | 31 | 0.9 | 8 | 25.8 | 0.2 | 2 | 6.5 | 0.1 |
| Medium range ($i-j >1$ & $i-j <5$) | 394 | 11.9 | 86 | 21.8 | 2.6 | 6 | 1.5 | 0.2 |
| Backbone-Backbone | 89 | 2.7 | 7 | 7.9 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 195 | 5.9 | 41 | 21.0 | 1.2 | 5 | 2.6 | 0.2 |
| Sidechain-Sidechain | 110 | 3.3 | 38 | 34.5 | 1.1 | 1 | 0.9 | 0.0 |
| Long range ($i-j \geq 5$) | 1220 | 36.8 | 204 | 16.7 | 6.1 | 29 | 2.4 | 0.9 |
| Backbone-Backbone | 273 | 8.2 | 24 | 8.8 | 0.7 | 7 | 2.6 | 0.2 |
| Backbone-Sidechain | 605 | 18.2 | 92 | 15.2 | 2.8 | 13 | 2.1 | 0.4 |
| Sidechain-Sidechain | 342 | 10.3 | 88 | 25.7 | 2.7 | 9 | 2.6 | 0.3 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 54 | 1.6 | 1 | 1.9 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 3318 | 100.0 | 610 | 18.4 | 18.4 | 115 | 3.5 | 3.5 |
| Backbone-Backbone | 801 | 24.1 | 56 | 7.0 | 1.7 | 13 | 1.6 | 0.4 |
| Backbone-Sidechain | 1802 | 54.3 | 376 | 20.9 | 11.3 | 65 | 3.6 | 2.0 |
| Sidechain-Sidechain | 715 | 21.5 | 178 | 24.9 | 5.4 | 37 | 5.2 | 1.1 |

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

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



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

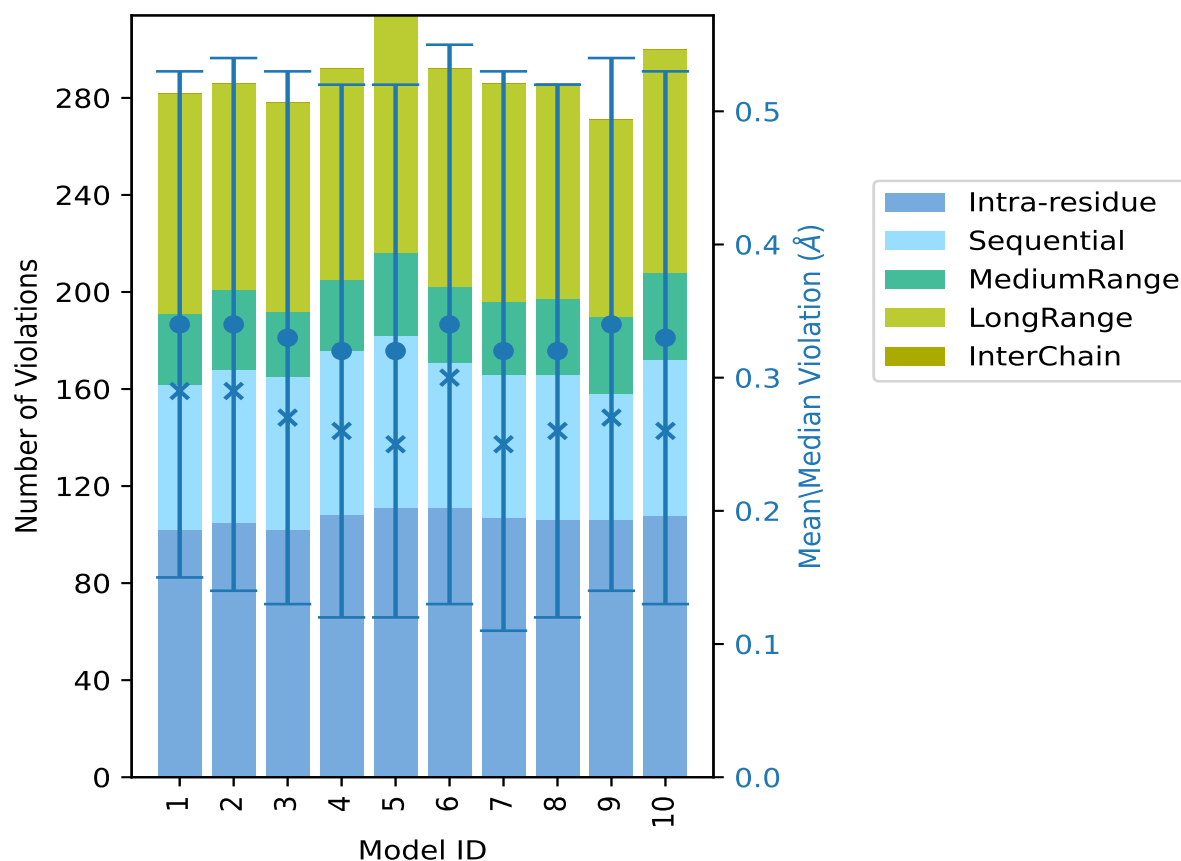
9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 102 | 60 | 29 | 91 | 0 | 282 | 0.34 | 1.07 | 0.19 | 0.29 |
| 2 | 105 | 63 | 33 | 85 | 0 | 286 | 0.34 | 1.01 | 0.2 | 0.29 |
| 3 | 102 | 63 | 27 | 86 | 0 | 278 | 0.33 | 0.98 | 0.2 | 0.27 |
| 4 | 108 | 68 | 29 | 87 | 0 | 292 | 0.32 | 1.08 | 0.2 | 0.26 |
| 5 | 111 | 71 | 34 | 98 | 0 | 314 | 0.32 | 1.11 | 0.2 | 0.25 |
| 6 | 111 | 60 | 31 | 90 | 0 | 292 | 0.34 | 1.18 | 0.21 | 0.3 |
| 7 | 107 | 59 | 30 | 90 | 0 | 286 | 0.32 | 1.07 | 0.21 | 0.25 |
| 8 | 106 | 60 | 31 | 89 | 0 | 286 | 0.32 | 1.06 | 0.2 | 0.26 |
| 9 | 106 | 52 | 32 | 81 | 0 | 271 | 0.34 | 1.08 | 0.2 | 0.27 |
| 10 | 108 | 64 | 36 | 92 | 0 | 300 | 0.33 | 0.93 | 0.2 | 0.26 |

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, 2655(IR:724, SQ:607, MR:308, LR:1016, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 48 | 19 | 33 | 56 | 0 | 156 | 1 | 10.0 |
| 11 | 31 | 15 | 33 | 0 | 90 | 2 | 20.0 |
| 15 | 8 | 6 | 21 | 0 | 50 | 3 | 30.0 |

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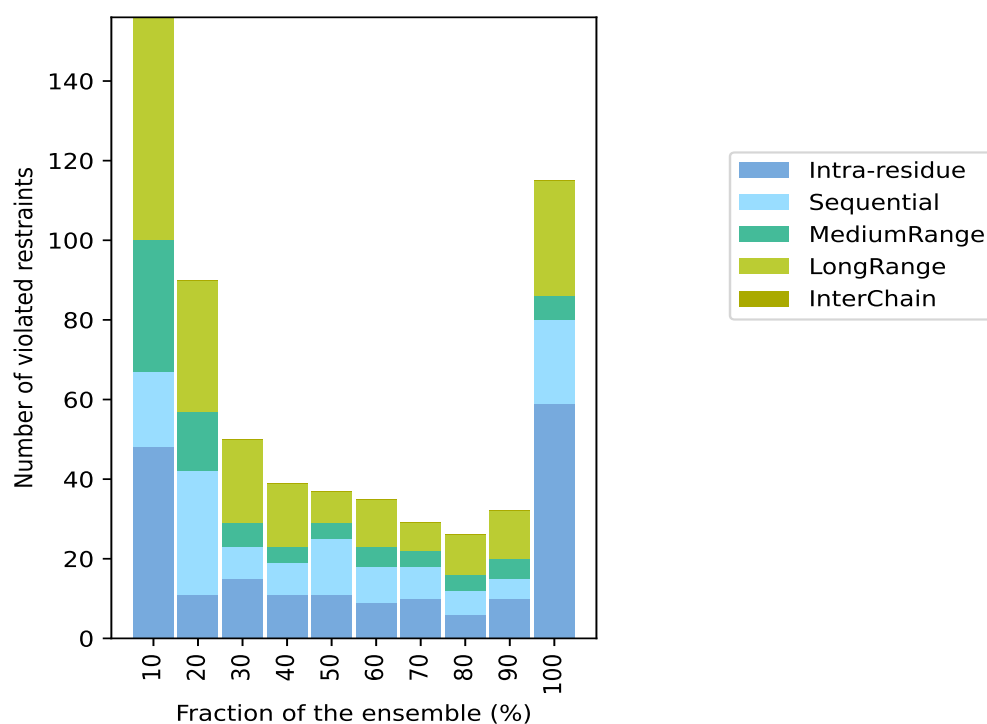
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 11 | 8 | 4 | 16 | 0 | 39 | 4 | 40.0 |
| 11 | 14 | 4 | 8 | 0 | 37 | 5 | 50.0 |
| 9 | 9 | 5 | 12 | 0 | 35 | 6 | 60.0 |
| 10 | 8 | 4 | 7 | 0 | 29 | 7 | 70.0 |
| 6 | 6 | 4 | 10 | 0 | 26 | 8 | 80.0 |
| 10 | 5 | 5 | 12 | 0 | 32 | 9 | 90.0 |
| 59 | 21 | 6 | 29 | 0 | 115 | 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 ⓘ

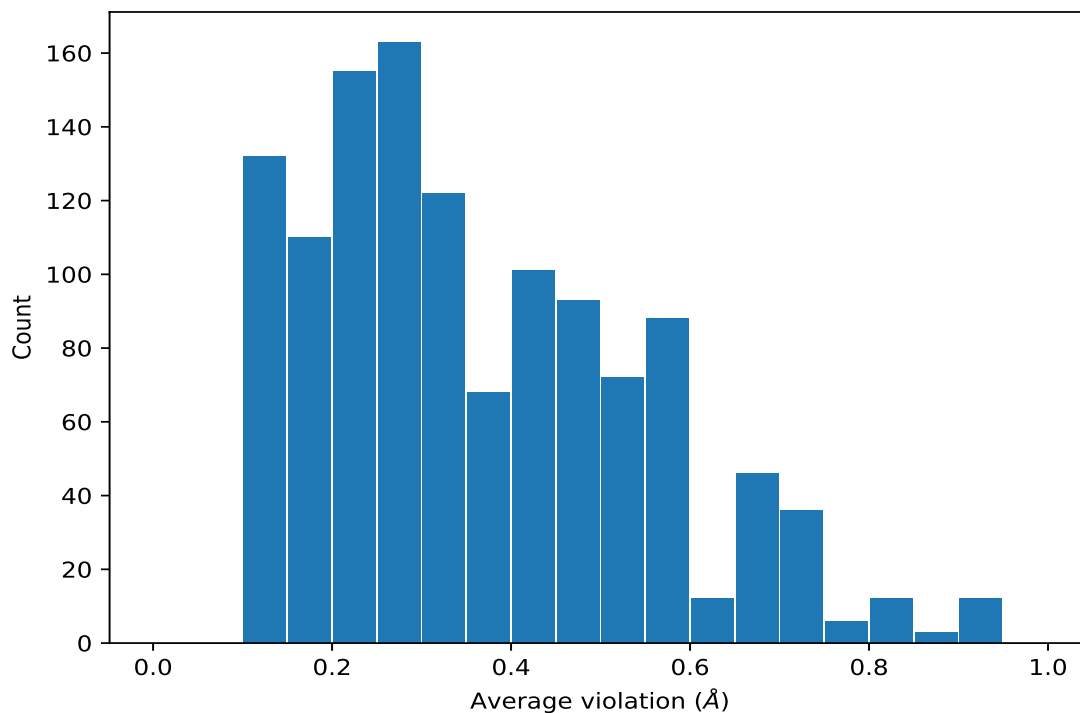


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 10 | 0.93 | 0.14 | 0.94 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 10 | 0.93 | 0.14 | 0.94 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 10 | 0.93 | 0.14 | 0.94 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 10 | 0.93 | 0.14 | 0.94 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 10 | 0.93 | 0.14 | 0.94 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 10 | 0.93 | 0.14 | 0.94 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 10 | 0.9 | 0.27 | 1.02 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 10 | 0.9 | 0.27 | 1.02 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 10 | 0.9 | 0.27 | 1.02 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 10 | 0.9 | 0.27 | 1.02 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 10 | 0.9 | 0.27 | 1.02 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 10 | 0.9 | 0.27 | 1.02 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 10 | 0.88 | 0.02 | 0.88 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 10 | 0.88 | 0.02 | 0.88 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 10 | 0.88 | 0.02 | 0.88 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 10 | 0.82 | 0.03 | 0.82 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 10 | 0.82 | 0.03 | 0.82 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 10 | 0.82 | 0.03 | 0.82 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 10 | 0.81 | 0.18 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 10 | 0.81 | 0.18 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 10 | 0.81 | 0.18 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 10 | 0.81 | 0.18 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 10 | 0.81 | 0.18 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 10 | 0.81 | 0.18 | 0.88 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 10 | 0.8 | 0.01 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 10 | 0.8 | 0.01 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 10 | 0.8 | 0.01 | 0.8 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 10 | 0.77 | 0.15 | 0.8 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 10 | 0.77 | 0.15 | 0.8 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 10 | 0.77 | 0.15 | 0.8 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 10 | 0.74 | 0.11 | 0.78 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 10 | 0.74 | 0.11 | 0.78 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 10 | 0.74 | 0.11 | 0.78 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 10 | 0.73 | 0.04 | 0.74 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 10 | 0.73 | 0.04 | 0.74 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 10 | 0.73 | 0.04 | 0.74 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 10 | 0.72 | 0.08 | 0.76 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 10 | 0.72 | 0.08 | 0.76 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 10 | 0.72 | 0.08 | 0.76 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 10 | 0.71 | 0.07 | 0.69 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 10 | 0.71 | 0.07 | 0.69 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 10 | 0.71 | 0.07 | 0.69 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 10 | 0.71 | 0.07 | 0.69 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 10 | 0.71 | 0.07 | 0.69 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 10 | 0.71 | 0.07 | 0.69 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 10 | 0.71 | 0.07 | 0.69 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 10 | 0.71 | 0.07 | 0.69 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 10 | 0.71 | 0.07 | 0.69 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 10 | 0.69 | 0.09 | 0.67 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 10 | 0.69 | 0.09 | 0.67 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 10 | 0.69 | 0.09 | 0.67 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 10 | 0.69 | 0.09 | 0.67 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 10 | 0.66 | 0.09 | 0.7 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 10 | 0.66 | 0.09 | 0.7 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 10 | 0.66 | 0.09 | 0.7 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 10 | 0.66 | 0.03 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 10 | 0.66 | 0.03 | 0.68 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 10 | 0.66 | 0.03 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 10 | 0.66 | 0.03 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 10 | 0.66 | 0.03 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 10 | 0.66 | 0.03 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 10 | 0.65 | 0.03 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 10 | 0.65 | 0.03 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 10 | 0.65 | 0.03 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 10 | 0.65 | 0.03 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 10 | 0.65 | 0.03 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 10 | 0.65 | 0.03 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 10 | 0.65 | 0.03 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 10 | 0.65 | 0.03 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 10 | 0.65 | 0.03 | 0.66 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 10 | 0.59 | 0.01 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 10 | 0.59 | 0.01 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 10 | 0.59 | 0.01 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 10 | 0.58 | 0.19 | 0.64 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 10 | 0.58 | 0.19 | 0.64 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 10 | 0.58 | 0.19 | 0.64 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 10 | 0.58 | 0.19 | 0.64 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 10 | 0.58 | 0.19 | 0.64 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 10 | 0.58 | 0.19 | 0.64 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 10 | 0.58 | 0.19 | 0.64 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 10 | 0.58 | 0.19 | 0.64 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 10 | 0.58 | 0.19 | 0.64 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 10 | 0.57 | 0.14 | 0.62 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 10 | 0.57 | 0.14 | 0.62 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 10 | 0.57 | 0.14 | 0.62 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 10 | 0.57 | 0.13 | 0.55 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 10 | 0.57 | 0.13 | 0.55 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 10 | 0.57 | 0.13 | 0.55 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 10 | 0.56 | 0.05 | 0.59 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 10 | 0.56 | 0.05 | 0.59 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 10 | 0.56 | 0.05 | 0.59 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 10 | 0.56 | 0.04 | 0.56 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 10 | 0.56 | 0.04 | 0.56 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 10 | 0.55 | 0.02 | 0.56 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 10 | 0.55 | 0.02 | 0.56 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 10 | 0.55 | 0.2 | 0.54 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 10 | 0.55 | 0.2 | 0.54 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 10 | 0.55 | 0.2 | 0.54 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 10 | 0.54 | 0.02 | 0.55 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 10 | 0.54 | 0.02 | 0.55 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 10 | 0.54 | 0.02 | 0.54 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 10 | 0.54 | 0.02 | 0.54 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 10 | 0.54 | 0.02 | 0.54 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 10 | 0.53 | 0.15 | 0.55 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 10 | 0.53 | 0.15 | 0.55 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 10 | 0.53 | 0.15 | 0.55 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 10 | 0.52 | 0.11 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 10 | 0.52 | 0.11 | 0.57 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 10 | 0.51 | 0.0 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 10 | 0.51 | 0.0 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 10 | 0.5 | 0.01 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 10 | 0.5 | 0.01 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 10 | 0.5 | 0.01 | 0.51 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 10 | 0.49 | 0.08 | 0.52 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 10 | 0.49 | 0.08 | 0.52 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 10 | 0.49 | 0.03 | 0.5 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 10 | 0.49 | 0.03 | 0.5 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 10 | 0.48 | 0.1 | 0.52 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 10 | 0.48 | 0.1 | 0.52 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 10 | 0.48 | 0.16 | 0.55 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 10 | 0.48 | 0.16 | 0.55 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 10 | 0.47 | 0.01 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 10 | 0.47 | 0.01 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 10 | 0.47 | 0.01 | 0.47 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 10 | 0.46 | 0.03 | 0.47 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 10 | 0.46 | 0.03 | 0.47 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 10 | 0.46 | 0.03 | 0.47 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 10 | 0.46 | 0.03 | 0.47 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 10 | 0.46 | 0.03 | 0.47 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 10 | 0.46 | 0.03 | 0.47 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 10 | 0.46 | 0.0 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 10 | 0.46 | 0.0 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 10 | 0.46 | 0.0 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 10 | 0.46 | 0.0 | 0.46 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 10 | 0.46 | 0.0 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 10 | 0.46 | 0.0 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 10 | 0.45 | 0.02 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 10 | 0.45 | 0.02 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 10 | 0.45 | 0.02 | 0.46 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 10 | 0.45 | 0.12 | 0.52 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 10 | 0.45 | 0.12 | 0.52 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 10 | 0.45 | 0.12 | 0.52 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 10 | 0.44 | 0.03 | 0.44 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 10 | 0.44 | 0.03 | 0.44 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 10 | 0.44 | 0.03 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 10 | 0.43 | 0.01 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 10 | 0.43 | 0.01 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 10 | 0.43 | 0.01 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 10 | 0.43 | 0.01 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 10 | 0.43 | 0.01 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 10 | 0.43 | 0.01 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 10 | 0.43 | 0.01 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 10 | 0.43 | 0.01 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 10 | 0.43 | 0.01 | 0.42 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 10 | 0.42 | 0.11 | 0.47 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 10 | 0.42 | 0.11 | 0.47 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 10 | 0.41 | 0.12 | 0.46 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 10 | 0.41 | 0.12 | 0.46 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 10 | 0.41 | 0.12 | 0.46 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 10 | 0.4 | 0.02 | 0.41 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 10 | 0.4 | 0.02 | 0.41 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 10 | 0.4 | 0.02 | 0.41 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 10 | 0.38 | 0.01 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 10 | 0.38 | 0.01 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 10 | 0.38 | 0.01 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 10 | 0.38 | 0.01 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 10 | 0.38 | 0.01 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 10 | 0.38 | 0.01 | 0.38 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 10 | 0.38 | 0.05 | 0.37 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 10 | 0.38 | 0.05 | 0.37 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 10 | 0.38 | 0.05 | 0.37 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 10 | 0.38 | 0.05 | 0.37 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 10 | 0.38 | 0.05 | 0.37 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 10 | 0.38 | 0.05 | 0.37 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 10 | 0.38 | 0.05 | 0.37 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 10 | 0.38 | 0.05 | 0.37 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 10 | 0.38 | 0.05 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 10 | 0.38 | 0.02 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 10 | 0.38 | 0.02 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 10 | 0.38 | 0.02 | 0.37 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 10 | 0.37 | 0.16 | 0.4 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 10 | 0.37 | 0.16 | 0.4 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 10 | 0.37 | 0.16 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 10 | 0.37 | 0.16 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 10 | 0.37 | 0.16 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 10 | 0.37 | 0.16 | 0.4 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 10 | 0.37 | 0.0 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 10 | 0.37 | 0.0 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 10 | 0.37 | 0.0 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 10 | 0.37 | 0.01 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 10 | 0.37 | 0.01 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 10 | 0.37 | 0.01 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 10 | 0.36 | 0.01 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 10 | 0.36 | 0.01 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 10 | 0.36 | 0.01 | 0.36 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 10 | 0.36 | 0.07 | 0.33 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 10 | 0.36 | 0.07 | 0.33 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 10 | 0.36 | 0.07 | 0.33 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 10 | 0.36 | 0.04 | 0.37 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 10 | 0.36 | 0.04 | 0.37 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 10 | 0.36 | 0.04 | 0.37 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 10 | 0.35 | 0.06 | 0.34 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 10 | 0.35 | 0.06 | 0.34 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 10 | 0.35 | 0.06 | 0.34 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 10 | 0.34 | 0.06 | 0.34 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 10 | 0.34 | 0.06 | 0.34 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 10 | 0.34 | 0.06 | 0.34 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 10 | 0.34 | 0.03 | 0.34 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 10 | 0.34 | 0.03 | 0.34 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 10 | 0.34 | 0.14 | 0.38 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 10 | 0.34 | 0.14 | 0.38 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 10 | 0.34 | 0.14 | 0.38 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 10 | 0.32 | 0.07 | 0.34 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 10 | 0.32 | 0.07 | 0.34 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 10 | 0.32 | 0.07 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 10 | 0.32 | 0.02 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 10 | 0.32 | 0.02 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 10 | 0.32 | 0.02 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 10 | 0.32 | 0.02 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 10 | 0.32 | 0.02 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 10 | 0.32 | 0.02 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 10 | 0.32 | 0.02 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 10 | 0.32 | 0.02 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 10 | 0.32 | 0.02 | 0.32 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 10 | 0.32 | 0.04 | 0.32 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 10 | 0.31 | 0.1 | 0.32 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 10 | 0.31 | 0.1 | 0.32 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 10 | 0.31 | 0.1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 10 | 0.31 | 0.01 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 10 | 0.31 | 0.01 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 10 | 0.31 | 0.01 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 10 | 0.31 | 0.01 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 10 | 0.31 | 0.01 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 10 | 0.31 | 0.01 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 10 | 0.31 | 0.01 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 10 | 0.31 | 0.01 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 10 | 0.31 | 0.01 | 0.31 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 10 | 0.3 | 0.07 | 0.32 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 10 | 0.3 | 0.07 | 0.32 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 10 | 0.3 | 0.07 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 10 | 0.3 | 0.07 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 10 | 0.3 | 0.07 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 10 | 0.3 | 0.07 | 0.32 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 10 | 0.3 | 0.07 | 0.32 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 10 | 0.3 | 0.07 | 0.32 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 10 | 0.3 | 0.07 | 0.32 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 10 | 0.3 | 0.12 | 0.37 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 10 | 0.3 | 0.12 | 0.37 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 10 | 0.3 | 0.12 | 0.37 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 10 | 0.3 | 0.03 | 0.29 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 10 | 0.3 | 0.03 | 0.29 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 10 | 0.3 | 0.03 | 0.29 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 10 | 0.3 | 0.17 | 0.29 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 10 | 0.3 | 0.17 | 0.29 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 10 | 0.3 | 0.17 | 0.29 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 10 | 0.3 | 0.17 | 0.29 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 10 | 0.3 | 0.17 | 0.29 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 10 | 0.3 | 0.17 | 0.29 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 10 | 0.28 | 0.01 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 10 | 0.28 | 0.01 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 10 | 0.28 | 0.01 | 0.28 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 10 | 0.26 | 0.12 | 0.27 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 10 | 0.26 | 0.12 | 0.27 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 10 | 0.26 | 0.01 | 0.26 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 10 | 0.26 | 0.04 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 10 | 0.26 | 0.04 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 10 | 0.26 | 0.04 | 0.25 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 10 | 0.26 | 0.02 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 10 | 0.26 | 0.02 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 10 | 0.26 | 0.02 | 0.26 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 10 | 0.25 | 0.04 | 0.26 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 10 | 0.25 | 0.01 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 10 | 0.24 | 0.02 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 10 | 0.24 | 0.02 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 10 | 0.24 | 0.02 | 0.25 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 10 | 0.24 | 0.03 | 0.26 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 10 | 0.24 | 0.03 | 0.24 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 10 | 0.23 | 0.07 | 0.24 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 10 | 0.23 | 0.04 | 0.22 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 10 | 0.23 | 0.04 | 0.22 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 10 | 0.23 | 0.04 | 0.22 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 10 | 0.22 | 0.02 | 0.22 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 10 | 0.22 | 0.02 | 0.23 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 10 | 0.22 | 0.02 | 0.23 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 10 | 0.22 | 0.02 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 10 | 0.22 | 0.02 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 10 | 0.22 | 0.02 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 10 | 0.22 | 0.02 | 0.22 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 10 | 0.22 | 0.02 | 0.21 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 10 | 0.21 | 0.04 | 0.22 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 10 | 0.21 | 0.04 | 0.22 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 10 | 0.21 | 0.04 | 0.22 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 10 | 0.21 | 0.04 | 0.22 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 10 | 0.21 | 0.04 | 0.22 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 10 | 0.21 | 0.04 | 0.22 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 10 | 0.21 | 0.04 | 0.22 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 10 | 0.21 | 0.04 | 0.22 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 10 | 0.21 | 0.04 | 0.22 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 10 | 0.2 | 0.01 | 0.19 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 10 | 0.2 | 0.0 | 0.2 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 10 | 0.2 | 0.06 | 0.18 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 10 | 0.2 | 0.02 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 10 | 0.19 | 0.01 | 0.19 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 10 | 0.19 | 0.03 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 10 | 0.18 | 0.01 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 10 | 0.18 | 0.01 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 10 | 0.18 | 0.01 | 0.18 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 10 | 0.18 | 0.04 | 0.18 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 10 | 0.18 | 0.02 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 10 | 0.18 | 0.01 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 10 | 0.18 | 0.01 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 10 | 0.18 | 0.01 | 0.18 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 10 | 0.18 | 0.02 | 0.18 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 10 | 0.18 | 0.01 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 10 | 0.18 | 0.01 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 10 | 0.18 | 0.01 | 0.17 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 10 | 0.18 | 0.03 | 0.18 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 10 | 0.17 | 0.05 | 0.16 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 10 | 0.17 | 0.05 | 0.16 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 10 | 0.17 | 0.05 | 0.16 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 10 | 0.17 | 0.01 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 10 | 0.17 | 0.01 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 10 | 0.17 | 0.01 | 0.17 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 10 | 0.17 | 0.03 | 0.18 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 10 | 0.16 | 0.0 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 10 | 0.16 | 0.0 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 10 | 0.16 | 0.0 | 0.16 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 10 | 0.16 | 0.0 | 0.16 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 10 | 0.15 | 0.03 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 10 | 0.15 | 0.0 | 0.15 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 10 | 0.15 | 0.02 | 0.16 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 10 | 0.15 | 0.02 | 0.15 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 10 | 0.14 | 0.02 | 0.15 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 10 | 0.13 | 0.01 | 0.13 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 10 | 0.13 | 0.02 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 10 | 0.12 | 0.0 | 0.12 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 10 | 0.12 | 0.01 | 0.12 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 9 | 0.73 | 0.01 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 9 | 0.73 | 0.01 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 9 | 0.73 | 0.01 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 9 | 0.73 | 0.01 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 9 | 0.73 | 0.01 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 9 | 0.73 | 0.01 | 0.73 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 9 | 0.7 | 0.02 | 0.7 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 9 | 0.7 | 0.02 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 9 | 0.7 | 0.02 | 0.7 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 9 | 0.67 | 0.11 | 0.73 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 9 | 0.67 | 0.11 | 0.73 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 9 | 0.67 | 0.11 | 0.73 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 9 | 0.66 | 0.02 | 0.66 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 9 | 0.66 | 0.02 | 0.66 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 9 | 0.66 | 0.02 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 9 | 0.62 | 0.06 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 9 | 0.62 | 0.06 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 9 | 0.62 | 0.06 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 9 | 0.62 | 0.06 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 9 | 0.62 | 0.06 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 9 | 0.62 | 0.06 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 9 | 0.62 | 0.06 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 9 | 0.62 | 0.06 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 9 | 0.62 | 0.06 | 0.63 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 9 | 0.6 | 0.21 | 0.64 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 9 | 0.6 | 0.21 | 0.64 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 9 | 0.6 | 0.21 | 0.64 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 9 | 0.6 | 0.25 | 0.72 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 9 | 0.6 | 0.25 | 0.72 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 9 | 0.6 | 0.25 | 0.72 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 9 | 0.6 | 0.25 | 0.72 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 9 | 0.57 | 0.11 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 9 | 0.57 | 0.11 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 9 | 0.57 | 0.11 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 9 | 0.57 | 0.11 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 9 | 0.57 | 0.11 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 9 | 0.57 | 0.11 | 0.64 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 9 | 0.57 | 0.06 | 0.57 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 9 | 0.57 | 0.06 | 0.57 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 9 | 0.57 | 0.06 | 0.57 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 9 | 0.54 | 0.05 | 0.54 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 9 | 0.54 | 0.05 | 0.54 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 9 | 0.49 | 0.17 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 9 | 0.49 | 0.17 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 9 | 0.49 | 0.17 | 0.62 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 9 | 0.48 | 0.11 | 0.53 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 9 | 0.48 | 0.11 | 0.53 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 9 | 0.48 | 0.11 | 0.53 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 9 | 0.48 | 0.1 | 0.51 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 9 | 0.48 | 0.1 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 9 | 0.48 | 0.1 | 0.51 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 9 | 0.45 | 0.0 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 9 | 0.45 | 0.0 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 9 | 0.45 | 0.0 | 0.45 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 9 | 0.45 | 0.09 | 0.49 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 9 | 0.45 | 0.09 | 0.49 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 9 | 0.4 | 0.1 | 0.44 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 9 | 0.4 | 0.1 | 0.44 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 9 | 0.4 | 0.1 | 0.44 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 9 | 0.4 | 0.19 | 0.39 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 9 | 0.4 | 0.19 | 0.39 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 9 | 0.4 | 0.19 | 0.39 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 9 | 0.4 | 0.03 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 9 | 0.4 | 0.03 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 9 | 0.4 | 0.03 | 0.41 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 9 | 0.4 | 0.13 | 0.47 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 9 | 0.4 | 0.13 | 0.47 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 9 | 0.4 | 0.13 | 0.47 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 9 | 0.38 | 0.05 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 9 | 0.38 | 0.05 | 0.39 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 9 | 0.35 | 0.1 | 0.32 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 9 | 0.35 | 0.1 | 0.32 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 9 | 0.35 | 0.1 | 0.32 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 9 | 0.34 | 0.04 | 0.32 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 9 | 0.34 | 0.03 | 0.33 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 9 | 0.34 | 0.03 | 0.33 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 9 | 0.34 | 0.03 | 0.33 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 9 | 0.34 | 0.11 | 0.32 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 9 | 0.34 | 0.11 | 0.32 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 9 | 0.34 | 0.11 | 0.32 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 9 | 0.27 | 0.1 | 0.24 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 9 | 0.25 | 0.01 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 9 | 0.25 | 0.01 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 9 | 0.25 | 0.01 | 0.25 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 9 | 0.22 | 0.08 | 0.23 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 9 | 0.22 | 0.08 | 0.23 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 9 | 0.22 | 0.08 | 0.23 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 9 | 0.17 | 0.03 | 0.17 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 9 | 0.17 | 0.03 | 0.17 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 9 | 0.17 | 0.03 | 0.17 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 9 | 0.15 | 0.02 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 9 | 0.14 | 0.01 | 0.13 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 9 | 0.12 | 0.02 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 9 | 0.12 | 0.02 | 0.12 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 9 | 0.12 | 0.02 | 0.12 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 9 | 0.12 | 0.02 | 0.12 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 8 | 0.58 | 0.2 | 0.58 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 8 | 0.58 | 0.2 | 0.58 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 8 | 0.58 | 0.2 | 0.58 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 8 | 0.58 | 0.2 | 0.58 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 8 | 0.57 | 0.29 | 0.64 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 8 | 0.57 | 0.29 | 0.64 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 8 | 0.57 | 0.29 | 0.64 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 8 | 0.57 | 0.29 | 0.64 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 8 | 0.53 | 0.19 | 0.48 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 8 | 0.53 | 0.19 | 0.48 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 8 | 0.53 | 0.19 | 0.48 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 8 | 0.53 | 0.19 | 0.48 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 8 | 0.53 | 0.19 | 0.48 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 8 | 0.53 | 0.19 | 0.48 |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 8 | 0.46 | 0.16 | 0.46 |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 8 | 0.46 | 0.16 | 0.46 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 8 | 0.46 | 0.16 | 0.46 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 8 | 0.45 | 0.01 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 8 | 0.45 | 0.01 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 8 | 0.45 | 0.01 | 0.45 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 8 | 0.44 | 0.11 | 0.42 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 8 | 0.44 | 0.11 | 0.42 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 8 | 0.44 | 0.11 | 0.42 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 8 | 0.44 | 0.11 | 0.42 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 8 | 0.44 | 0.11 | 0.42 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 8 | 0.44 | 0.11 | 0.42 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 8 | 0.43 | 0.2 | 0.44 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 8 | 0.43 | 0.2 | 0.44 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 8 | 0.43 | 0.2 | 0.44 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 8 | 0.43 | 0.2 | 0.44 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 8 | 0.43 | 0.2 | 0.44 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 8 | 0.43 | 0.2 | 0.44 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 8 | 0.34 | 0.15 | 0.38 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 8 | 0.34 | 0.15 | 0.38 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 8 | 0.31 | 0.12 | 0.34 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 8 | 0.31 | 0.12 | 0.34 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 8 | 0.31 | 0.04 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 8 | 0.31 | 0.04 | 0.32 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 8 | 0.29 | 0.15 | 0.26 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 8 | 0.29 | 0.15 | 0.26 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 8 | 0.29 | 0.15 | 0.26 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 8 | 0.29 | 0.15 | 0.26 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 8 | 0.29 | 0.15 | 0.26 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 8 | 0.29 | 0.15 | 0.26 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 8 | 0.29 | 0.12 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 8 | 0.29 | 0.12 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 8 | 0.29 | 0.12 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 8 | 0.29 | 0.12 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 8 | 0.29 | 0.12 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 8 | 0.29 | 0.12 | 0.3 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 8 | 0.25 | 0.06 | 0.26 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 8 | 0.25 | 0.06 | 0.26 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 8 | 0.25 | 0.03 | 0.26 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 8 | 0.25 | 0.03 | 0.26 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 8 | 0.25 | 0.03 | 0.26 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 8 | 0.21 | 0.02 | 0.2 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 8 | 0.2 | 0.04 | 0.2 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 8 | 0.2 | 0.04 | 0.2 |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 8 | 0.2 | 0.04 | 0.2 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 8 | 0.2 | 0.06 | 0.18 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 8 | 0.2 | 0.03 | 0.2 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 8 | 0.16 | 0.03 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 8 | 0.16 | 0.03 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 8 | 0.16 | 0.03 | 0.16 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 8 | 0.14 | 0.03 | 0.14 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 8 | 0.14 | 0.06 | 0.11 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 8 | 0.14 | 0.06 | 0.11 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 8 | 0.14 | 0.06 | 0.11 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 8 | 0.13 | 0.02 | 0.13 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 8 | 0.12 | 0.01 | 0.12 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 8 | 0.12 | 0.02 | 0.12 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 8 | 0.11 | 0.0 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 8 | 0.11 | 0.0 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 8 | 0.11 | 0.0 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 8 | 0.11 | 0.0 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 8 | 0.11 | 0.0 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 8 | 0.11 | 0.0 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 8 | 0.11 | 0.0 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 8 | 0.11 | 0.0 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 8 | 0.11 | 0.0 | 0.11 |
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD11 | 7 | 0.53 | 0.01 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD12 | 7 | 0.53 | 0.01 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD13 | 7 | 0.53 | 0.01 | 0.53 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG11 | 7 | 0.5 | 0.1 | 0.53 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG12 | 7 | 0.5 | 0.1 | 0.53 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG13 | 7 | 0.5 | 0.1 | 0.53 |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA | 7 | 0.49 | 0.01 | 0.49 |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA | 7 | 0.49 | 0.01 | 0.49 |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H | 7 | 0.49 | 0.07 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H | 7 | 0.49 | 0.07 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H | 7 | 0.49 | 0.07 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H | 7 | 0.49 | 0.07 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H | 7 | 0.49 | 0.07 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H | 7 | 0.49 | 0.07 | 0.51 |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H | 7 | 0.46 | 0.03 | 0.45 |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H | 7 | 0.46 | 0.03 | 0.45 |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H | 7 | 0.46 | 0.03 | 0.45 |
| (1,1475) | 1:95:A:PHE:HB2 | 1:96:A:SER:H | 7 | 0.4 | 0.03 | 0.4 |
| (1,1475) | 1:95:A:PHE:HB3 | 1:96:A:SER:H | 7 | 0.4 | 0.03 | 0.4 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 7 | 0.4 | 0.08 | 0.45 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 7 | 0.4 | 0.08 | 0.45 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 7 | 0.4 | 0.08 | 0.45 |
| (1,1556) | 1:103:A:SER:HA | 1:104:A:LEU:HB3 | 7 | 0.33 | 0.02 | 0.33 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG21 | 7 | 0.32 | 0.05 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG22 | 7 | 0.32 | 0.05 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG23 | 7 | 0.32 | 0.05 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG21 | 7 | 0.32 | 0.05 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG22 | 7 | 0.32 | 0.05 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG23 | 7 | 0.32 | 0.05 | 0.31 |
| (1,2327) | 1:171:A:LEU:HG | 1:171:A:LEU:H | 7 | 0.31 | 0.05 | 0.32 |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H | 7 | 0.31 | 0.18 | 0.23 |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H | 7 | 0.31 | 0.18 | 0.23 |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H | 7 | 0.31 | 0.18 | 0.23 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE1 | 7 | 0.31 | 0.14 | 0.31 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE2 | 7 | 0.31 | 0.14 | 0.31 |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H | 7 | 0.3 | 0.17 | 0.24 |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H | 7 | 0.3 | 0.17 | 0.24 |
| (1,1338) | 1:85:A:TYR:HD1 | 1:86:A:GLU:H | 7 | 0.3 | 0.09 | 0.3 |
| (1,1338) | 1:85:A:TYR:HD2 | 1:86:A:GLU:H | 7 | 0.3 | 0.09 | 0.3 |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H | 7 | 0.28 | 0.06 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H | 7 | 0.28 | 0.06 | 0.28 |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H | 7 | 0.27 | 0.03 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H | 7 | 0.27 | 0.03 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H | 7 | 0.27 | 0.03 | 0.27 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE1 | 7 | 0.24 | 0.1 | 0.22 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE2 | 7 | 0.24 | 0.1 | 0.22 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD11 | 7 | 0.24 | 0.02 | 0.24 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD12 | 7 | 0.24 | 0.02 | 0.24 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD13 | 7 | 0.24 | 0.02 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 7 | 0.24 | 0.02 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 7 | 0.24 | 0.02 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 7 | 0.24 | 0.02 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 7 | 0.24 | 0.02 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 7 | 0.24 | 0.02 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 7 | 0.24 | 0.02 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 7 | 0.24 | 0.02 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 7 | 0.24 | 0.02 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 7 | 0.24 | 0.02 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD21 | 7 | 0.23 | 0.06 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD22 | 7 | 0.23 | 0.06 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD23 | 7 | 0.23 | 0.06 | 0.23 |
| (2,178) | 1:36:A:ALA:H | 1:37:A:GLY:H | 7 | 0.21 | 0.08 | 0.21 |
| (1,1505) | 1:98:A:THR:HA | 1:100:A:ALA:H | 7 | 0.16 | 0.03 | 0.16 |
| (1,914) | 1:69:A:GLN:HG3 | 1:69:A:GLN:H | 7 | 0.16 | 0.04 | 0.16 |
| (1,857) | 1:66:A:ASN:HD22 | 1:174:A:ILE:H | 7 | 0.15 | 0.03 | 0.16 |
| (1,1371) | 1:86:A:GLU:H | 1:134:A:TRP:HE1 | 7 | 0.14 | 0.03 | 0.13 |
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2 | 7 | 0.13 | 0.05 | 0.11 |
| (1,548) | 1:50:A:TRP:HB3 | 1:50:A:TRP:H | 7 | 0.12 | 0.01 | 0.12 |
| (1,1127) | 1:78:A:GLN:H | 1:104:A:LEU:H | 7 | 0.12 | 0.02 | 0.13 |
| (1,1618) | 1:108:A:SER:H | 1:109:A:ALA:H | 7 | 0.1 | 0.0 | 0.1 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 6 | 0.75 | 0.03 | 0.75 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 6 | 0.75 | 0.03 | 0.75 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 6 | 0.75 | 0.03 | 0.75 |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H | 6 | 0.49 | 0.01 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H | 6 | 0.49 | 0.01 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H | 6 | 0.49 | 0.01 | 0.49 |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H | 6 | 0.47 | 0.1 | 0.51 |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H | 6 | 0.47 | 0.1 | 0.51 |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H | 6 | 0.46 | 0.01 | 0.46 |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H | 6 | 0.46 | 0.01 | 0.46 |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H | 6 | 0.46 | 0.01 | 0.46 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 6 | 0.46 | 0.03 | 0.45 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 6 | 0.46 | 0.03 | 0.45 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 6 | 0.46 | 0.03 | 0.45 |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H | 6 | 0.4 | 0.09 | 0.42 |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H | 6 | 0.4 | 0.09 | 0.42 |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H | 6 | 0.4 | 0.09 | 0.42 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG21 | 6 | 0.4 | 0.16 | 0.36 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG22 | 6 | 0.4 | 0.16 | 0.36 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG23 | 6 | 0.4 | 0.16 | 0.36 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG21 | 6 | 0.4 | 0.16 | 0.36 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG22 | 6 | 0.4 | 0.16 | 0.36 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG23 | 6 | 0.4 | 0.16 | 0.36 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD21 | 6 | 0.35 | 0.1 | 0.38 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD22 | 6 | 0.35 | 0.1 | 0.38 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD1 | 6 | 0.3 | 0.12 | 0.28 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD2 | 6 | 0.3 | 0.12 | 0.28 |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H | 6 | 0.3 | 0.18 | 0.24 |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H | 6 | 0.3 | 0.18 | 0.24 |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H | 6 | 0.3 | 0.18 | 0.24 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 6 | 0.3 | 0.1 | 0.34 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 6 | 0.3 | 0.1 | 0.34 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 6 | 0.3 | 0.1 | 0.34 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 6 | 0.3 | 0.1 | 0.34 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 6 | 0.3 | 0.1 | 0.34 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 6 | 0.3 | 0.1 | 0.34 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG21 | 6 | 0.29 | 0.13 | 0.27 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG22 | 6 | 0.29 | 0.13 | 0.27 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG23 | 6 | 0.29 | 0.13 | 0.27 |
| (1,873) | 1:67:A:ALA:HB1 | 1:68:A:GLU:H | 6 | 0.25 | 0.03 | 0.25 |
| (1,873) | 1:67:A:ALA:HB2 | 1:68:A:GLU:H | 6 | 0.25 | 0.03 | 0.25 |
| (1,873) | 1:67:A:ALA:HB3 | 1:68:A:GLU:H | 6 | 0.25 | 0.03 | 0.25 |
| (2,714) | 1:141:A:LYS:HD2 | 1:142:A:ILE:H | 6 | 0.24 | 0.06 | 0.22 |
| (2,714) | 1:141:A:LYS:HD3 | 1:142:A:ILE:H | 6 | 0.24 | 0.06 | 0.22 |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H | 6 | 0.23 | 0.07 | 0.22 |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H | 6 | 0.23 | 0.07 | 0.22 |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H | 6 | 0.23 | 0.07 | 0.22 |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H | 6 | 0.23 | 0.01 | 0.23 |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H | 6 | 0.23 | 0.01 | 0.23 |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H | 6 | 0.23 | 0.01 | 0.23 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD21 | 6 | 0.23 | 0.04 | 0.24 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD22 | 6 | 0.23 | 0.04 | 0.24 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD23 | 6 | 0.23 | 0.04 | 0.24 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE1 | 6 | 0.22 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE2 | 6 | 0.22 | 0.08 | 0.22 |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H | 6 | 0.21 | 0.07 | 0.19 |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H | 6 | 0.21 | 0.07 | 0.19 |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H | 6 | 0.21 | 0.07 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.11 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 6 | 0.2 | 0.02 | 0.2 |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H | 6 | 0.18 | 0.07 | 0.17 |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H | 6 | 0.18 | 0.07 | 0.17 |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H | 6 | 0.18 | 0.07 | 0.17 |
| (1,1774) | 1:121:A:LEU:HB3 | 1:121:A:LEU:H | 6 | 0.18 | 0.02 | 0.18 |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H | 6 | 0.18 | 0.02 | 0.18 |
| (1,235) | 1:32:A:ILE:HG22 | 1:33:A:THR:H | 6 | 0.18 | 0.02 | 0.18 |
| (1,235) | 1:32:A:ILE:HG23 | 1:33:A:THR:H | 6 | 0.18 | 0.02 | 0.18 |
| (1,845) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA | 6 | 0.16 | 0.02 | 0.17 |
| (1,1723) | 1:116:A:GLU:HG2 | 1:116:A:GLU:H | 6 | 0.16 | 0.05 | 0.12 |
| (1,1723) | 1:116:A:GLU:HG3 | 1:116:A:GLU:H | 6 | 0.16 | 0.05 | 0.12 |
| (1,1128) | 1:78:A:GLN:H | 1:158:A:ALA:HA | 6 | 0.16 | 0.02 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,554) | 1:50:A:TRP:HD1 | 1:50:A:TRP:H | 6 | 0.15 | 0.02 | 0.15 |
| (1,2260) | 1:163:A:LYS:H | 1:168:A:PHE:HZ | 6 | 0.14 | 0.03 | 0.14 |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H | 6 | 0.14 | 0.01 | 0.14 |
| (1,426) | 1:46:A:TYR:HA | 1:156:A:PHE:HA | 6 | 0.13 | 0.02 | 0.13 |
| (1,761) | 1:63:A:THR:H | 1:175:A:PHE:HA | 6 | 0.12 | 0.02 | 0.12 |
| (1,795) | 1:64:A:LEU:HG | 1:67:A:ALA:HA | 6 | 0.11 | 0.01 | 0.12 |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H | 6 | 0.11 | 0.02 | 0.1 |
| (1,2459) | 1:182:A:VAL:HB | 1:183:A:GLY:H | 6 | 0.1 | 0.0 | 0.11 |
| (1,282) | 1:35:A:ALA:HB1 | 1:36:A:ALA:H | 5 | 0.6 | 0.06 | 0.57 |
| (1,282) | 1:35:A:ALA:HB2 | 1:36:A:ALA:H | 5 | 0.6 | 0.06 | 0.57 |
| (1,282) | 1:35:A:ALA:HB3 | 1:36:A:ALA:H | 5 | 0.6 | 0.06 | 0.57 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB2 | 5 | 0.58 | 0.36 | 0.79 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB3 | 5 | 0.58 | 0.36 | 0.79 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB2 | 5 | 0.58 | 0.36 | 0.79 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB3 | 5 | 0.58 | 0.36 | 0.79 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB2 | 5 | 0.58 | 0.36 | 0.79 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB3 | 5 | 0.58 | 0.36 | 0.79 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD21 | 5 | 0.55 | 0.2 | 0.65 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD22 | 5 | 0.55 | 0.2 | 0.65 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD23 | 5 | 0.55 | 0.2 | 0.65 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD11 | 5 | 0.55 | 0.3 | 0.52 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD12 | 5 | 0.55 | 0.3 | 0.52 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD13 | 5 | 0.55 | 0.3 | 0.52 |
| (2,631) | 1:122:A:TYR:HD1 | 1:124:A:ASP:H | 5 | 0.5 | 0.01 | 0.5 |
| (2,631) | 1:122:A:TYR:HD2 | 1:124:A:ASP:H | 5 | 0.5 | 0.01 | 0.5 |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3 | 5 | 0.43 | 0.16 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3 | 5 | 0.43 | 0.16 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3 | 5 | 0.43 | 0.16 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3 | 5 | 0.43 | 0.16 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3 | 5 | 0.43 | 0.16 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3 | 5 | 0.43 | 0.16 | 0.47 |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA | 5 | 0.43 | 0.11 | 0.51 |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA | 5 | 0.43 | 0.11 | 0.51 |
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA | 5 | 0.43 | 0.11 | 0.51 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD11 | 5 | 0.41 | 0.01 | 0.41 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD12 | 5 | 0.41 | 0.01 | 0.41 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD13 | 5 | 0.41 | 0.01 | 0.41 |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H | 5 | 0.39 | 0.1 | 0.47 |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H | 5 | 0.39 | 0.1 | 0.47 |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H | 5 | 0.39 | 0.1 | 0.47 |
| (1,11) | 1:20:A:SER:HB2 | 1:21:A:GLU:H | 5 | 0.34 | 0.09 | 0.39 |
| (1,11) | 1:20:A:SER:HB3 | 1:21:A:GLU:H | 5 | 0.34 | 0.09 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE1 | 5 | 0.33 | 0.09 | 0.29 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE2 | 5 | 0.33 | 0.09 | 0.29 |
| (1,166) | 1:29:A:LEU:HD11 | 1:175:A:PHE:H | 5 | 0.31 | 0.16 | 0.29 |
| (1,166) | 1:29:A:LEU:HD12 | 1:175:A:PHE:H | 5 | 0.31 | 0.16 | 0.29 |
| (1,166) | 1:29:A:LEU:HD13 | 1:175:A:PHE:H | 5 | 0.31 | 0.16 | 0.29 |
| (1,2054) | 1:145:A:TYR:HD1 | 1:146:A:ASN:H | 5 | 0.3 | 0.09 | 0.34 |
| (1,2054) | 1:145:A:TYR:HD2 | 1:146:A:ASN:H | 5 | 0.3 | 0.09 | 0.34 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD11 | 5 | 0.28 | 0.2 | 0.19 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD12 | 5 | 0.28 | 0.2 | 0.19 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD13 | 5 | 0.28 | 0.2 | 0.19 |
| (2,534) | 1:85:A:TYR:HE1 | 1:151:A:VAL:H | 5 | 0.28 | 0.15 | 0.19 |
| (2,534) | 1:85:A:TYR:HE2 | 1:151:A:VAL:H | 5 | 0.28 | 0.15 | 0.19 |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB | 5 | 0.27 | 0.11 | 0.27 |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB | 5 | 0.27 | 0.11 | 0.27 |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB | 5 | 0.27 | 0.11 | 0.27 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 5 | 0.27 | 0.27 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 5 | 0.27 | 0.27 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 5 | 0.27 | 0.27 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 5 | 0.27 | 0.27 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 5 | 0.27 | 0.27 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 5 | 0.27 | 0.27 | 0.13 |
| (1,915) | 1:69:A:GLN:HG3 | 1:70:A:LEU:H | 5 | 0.24 | 0.04 | 0.23 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD1 | 5 | 0.24 | 0.07 | 0.23 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD2 | 5 | 0.24 | 0.07 | 0.23 |
| (1,909) | 1:69:A:GLN:HB2 | 1:70:A:LEU:H | 5 | 0.21 | 0.06 | 0.2 |
| (1,922) | 1:70:A:LEU:HD11 | 1:70:A:LEU:H | 5 | 0.19 | 0.08 | 0.16 |
| (1,922) | 1:70:A:LEU:HD12 | 1:70:A:LEU:H | 5 | 0.19 | 0.08 | 0.16 |
| (1,922) | 1:70:A:LEU:HD13 | 1:70:A:LEU:H | 5 | 0.19 | 0.08 | 0.16 |
| (1,455) | 1:47:A:ALA:HB1 | 1:48:A:ILE:H | 5 | 0.19 | 0.07 | 0.16 |
| (1,455) | 1:47:A:ALA:HB2 | 1:48:A:ILE:H | 5 | 0.19 | 0.07 | 0.16 |
| (1,455) | 1:47:A:ALA:HB3 | 1:48:A:ILE:H | 5 | 0.19 | 0.07 | 0.16 |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H | 5 | 0.18 | 0.06 | 0.15 |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H | 5 | 0.18 | 0.06 | 0.15 |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H | 5 | 0.18 | 0.06 | 0.15 |
| (1,849) | 1:66:A:ASN:HD22 | 1:66:A:ASN:H | 5 | 0.18 | 0.01 | 0.18 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG21 | 5 | 0.18 | 0.05 | 0.17 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG22 | 5 | 0.18 | 0.05 | 0.17 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG23 | 5 | 0.18 | 0.05 | 0.17 |
| (1,292) | 1:37:A:GLY:HA2 | 1:37:A:GLY:H | 5 | 0.17 | 0.05 | 0.15 |
| (1,894) | 1:68:A:GLU:H | 1:69:A:GLN:H | 5 | 0.15 | 0.03 | 0.15 |
| (1,541) | 1:50:A:TRP:HA | 1:51:A:ILE:HB | 5 | 0.15 | 0.03 | 0.17 |
| (2,205) | 1:39:A:GLN:HB3 | 1:39:A:GLN:HE21 | 5 | 0.14 | 0.0 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1363) | 1:86:A:GLU:HG3 | 1:86:A:GLU:H | 5 | 0.13 | 0.01 | 0.13 |
| (1,2258) | 1:163:A:LYS:HG2 | 1:163:A:LYS:H | 5 | 0.13 | 0.01 | 0.14 |
| (1,683) | 1:60:A:LEU:HG | 1:60:A:LEU:H | 5 | 0.13 | 0.01 | 0.12 |
| (1,1778) | 1:121:A:LEU:HG | 1:121:A:LEU:H | 5 | 0.12 | 0.01 | 0.12 |
| (1,1379) | 1:87:A:THR:HA | 1:134:A:TRP:HE3 | 5 | 0.12 | 0.01 | 0.12 |
| (1,643) | 1:57:A:ASP:HB2 | 1:115:A:LYS:H | 5 | 0.12 | 0.01 | 0.12 |
| (1,1974) | 1:138:A:GLU:H | 1:139:A:PRO:HD2 | 5 | 0.11 | 0.0 | 0.11 |
| (1,2275) | 1:167:A:LEU:HA | 1:168:A:PHE:H | 5 | 0.1 | 0.0 | 0.1 |
| (2,7) | 1:16:A:ALA:HB1 | 1:18:A:ALA:H | 4 | 0.65 | 0.09 | 0.64 |
| (2,7) | 1:16:A:ALA:HB2 | 1:18:A:ALA:H | 4 | 0.65 | 0.09 | 0.64 |
| (2,7) | 1:16:A:ALA:HB3 | 1:18:A:ALA:H | 4 | 0.65 | 0.09 | 0.64 |
| (1,923) | 1:70:A:LEU:HD11 | 1:71:A:LYS:H | 4 | 0.6 | 0.03 | 0.6 |
| (1,923) | 1:70:A:LEU:HD12 | 1:71:A:LYS:H | 4 | 0.6 | 0.03 | 0.6 |
| (1,923) | 1:70:A:LEU:HD13 | 1:71:A:LYS:H | 4 | 0.6 | 0.03 | 0.6 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD11 | 4 | 0.59 | 0.03 | 0.6 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD12 | 4 | 0.59 | 0.03 | 0.6 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD13 | 4 | 0.59 | 0.03 | 0.6 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD11 | 4 | 0.59 | 0.03 | 0.6 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD12 | 4 | 0.59 | 0.03 | 0.6 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD13 | 4 | 0.59 | 0.03 | 0.6 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE1 | 4 | 0.52 | 0.22 | 0.54 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE2 | 4 | 0.52 | 0.22 | 0.54 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE1 | 4 | 0.52 | 0.22 | 0.54 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE2 | 4 | 0.52 | 0.22 | 0.54 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE1 | 4 | 0.52 | 0.22 | 0.54 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE2 | 4 | 0.52 | 0.22 | 0.54 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1 | 4 | 0.5 | 0.2 | 0.5 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2 | 4 | 0.5 | 0.2 | 0.5 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1 | 4 | 0.5 | 0.2 | 0.5 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2 | 4 | 0.5 | 0.2 | 0.5 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1 | 4 | 0.5 | 0.2 | 0.5 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2 | 4 | 0.5 | 0.2 | 0.5 |
| (2,94) | 1:23:A:ILE:HD11 | 1:53:A:ASP:H | 4 | 0.48 | 0.23 | 0.53 |
| (2,94) | 1:23:A:ILE:HD12 | 1:53:A:ASP:H | 4 | 0.48 | 0.23 | 0.53 |
| (2,94) | 1:23:A:ILE:HD13 | 1:53:A:ASP:H | 4 | 0.48 | 0.23 | 0.53 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB1 | 4 | 0.48 | 0.18 | 0.44 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB2 | 4 | 0.48 | 0.18 | 0.44 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB3 | 4 | 0.48 | 0.18 | 0.44 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB1 | 4 | 0.48 | 0.18 | 0.44 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB2 | 4 | 0.48 | 0.18 | 0.44 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB3 | 4 | 0.48 | 0.18 | 0.44 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE1 | 4 | 0.46 | 0.09 | 0.5 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE2 | 4 | 0.46 | 0.09 | 0.5 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG21 | 4 | 0.46 | 0.02 | 0.45 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG22 | 4 | 0.46 | 0.02 | 0.45 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG23 | 4 | 0.46 | 0.02 | 0.45 |
| (1,1090) | 1:77:A:LEU:HD11 | 1:79:A:ILE:H | 4 | 0.42 | 0.07 | 0.42 |
| (1,1090) | 1:77:A:LEU:HD12 | 1:79:A:ILE:H | 4 | 0.42 | 0.07 | 0.42 |
| (1,1090) | 1:77:A:LEU:HD13 | 1:79:A:ILE:H | 4 | 0.42 | 0.07 | 0.42 |
| (1,1090) | 1:77:A:LEU:HD21 | 1:79:A:ILE:H | 4 | 0.42 | 0.07 | 0.42 |
| (1,1090) | 1:77:A:LEU:HD22 | 1:79:A:ILE:H | 4 | 0.42 | 0.07 | 0.42 |
| (1,1090) | 1:77:A:LEU:HD23 | 1:79:A:ILE:H | 4 | 0.42 | 0.07 | 0.42 |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H | 4 | 0.4 | 0.17 | 0.45 |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H | 4 | 0.4 | 0.17 | 0.45 |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H | 4 | 0.4 | 0.17 | 0.45 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG2 | 4 | 0.39 | 0.12 | 0.42 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG3 | 4 | 0.39 | 0.12 | 0.42 |
| (1,289) | 1:37:A:GLY:HA3 | 1:37:A:GLY:H | 4 | 0.37 | 0.09 | 0.39 |
| (1,1707) | 1:115:A:LYS:HG2 | 1:116:A:GLU:H | 4 | 0.36 | 0.01 | 0.36 |
| (1,1707) | 1:115:A:LYS:HG3 | 1:116:A:GLU:H | 4 | 0.36 | 0.01 | 0.36 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD11 | 4 | 0.35 | 0.15 | 0.32 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD12 | 4 | 0.35 | 0.15 | 0.32 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD13 | 4 | 0.35 | 0.15 | 0.32 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE1 | 4 | 0.34 | 0.03 | 0.34 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE2 | 4 | 0.34 | 0.03 | 0.34 |
| (2,397) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HA | 4 | 0.31 | 0.15 | 0.3 |
| (2,397) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HA | 4 | 0.31 | 0.15 | 0.3 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD11 | 4 | 0.3 | 0.04 | 0.29 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD12 | 4 | 0.3 | 0.04 | 0.29 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD13 | 4 | 0.3 | 0.04 | 0.29 |
| (1,1483) | 1:95:A:PHE:HE1 | 1:116:A:GLU:HB3 | 4 | 0.27 | 0.05 | 0.29 |
| (1,1483) | 1:95:A:PHE:HE2 | 1:116:A:GLU:HB3 | 4 | 0.27 | 0.05 | 0.29 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG21 | 4 | 0.24 | 0.04 | 0.26 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG22 | 4 | 0.24 | 0.04 | 0.26 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG23 | 4 | 0.24 | 0.04 | 0.26 |
| (1,597) | 1:53:A:ASP:HB2 | 1:54:A:GLN:H | 4 | 0.22 | 0.1 | 0.21 |
| (1,597) | 1:53:A:ASP:HB3 | 1:54:A:GLN:H | 4 | 0.22 | 0.1 | 0.21 |
| (1,2154) | 1:156:A:PHE:HD1 | 1:156:A:PHE:H | 4 | 0.22 | 0.01 | 0.22 |
| (1,2154) | 1:156:A:PHE:HD2 | 1:156:A:PHE:H | 4 | 0.22 | 0.01 | 0.22 |
| (1,908) | 1:69:A:GLN:HB3 | 1:70:A:LEU:H | 4 | 0.2 | 0.05 | 0.18 |
| (1,911) | 1:69:A:GLN:HE22 | 1:70:A:LEU:H | 4 | 0.2 | 0.03 | 0.2 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG21 | 4 | 0.2 | 0.01 | 0.2 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG22 | 4 | 0.2 | 0.01 | 0.2 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG23 | 4 | 0.2 | 0.01 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,755) | 1:63:A:THR:HG21 | 1:108:A:SER:HA | 4 | 0.19 | 0.08 | 0.19 |
| (1,755) | 1:63:A:THR:HG22 | 1:108:A:SER:HA | 4 | 0.19 | 0.08 | 0.19 |
| (1,755) | 1:63:A:THR:HG23 | 1:108:A:SER:HA | 4 | 0.19 | 0.08 | 0.19 |
| (1,2455) | 1:182:A:VAL:HA | 1:182:A:VAL:HB | 4 | 0.17 | 0.0 | 0.17 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG21 | 4 | 0.16 | 0.01 | 0.16 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG22 | 4 | 0.16 | 0.01 | 0.16 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG23 | 4 | 0.16 | 0.01 | 0.16 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG21 | 4 | 0.16 | 0.02 | 0.15 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG22 | 4 | 0.16 | 0.02 | 0.15 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG23 | 4 | 0.16 | 0.02 | 0.15 |
| (1,48) | 1:24:A:ASP:HB3 | 1:50:A:TRP:HD1 | 4 | 0.15 | 0.03 | 0.15 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG21 | 4 | 0.14 | 0.03 | 0.15 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG22 | 4 | 0.14 | 0.03 | 0.15 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG23 | 4 | 0.14 | 0.03 | 0.15 |
| (1,831) | 1:66:A:ASN:HA | 1:174:A:ILE:HB | 4 | 0.14 | 0.01 | 0.14 |
| (1,854) | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3 | 4 | 0.14 | 0.03 | 0.13 |
| (1,77) | 1:25:A:VAL:HG11 | 1:25:A:VAL:H | 4 | 0.14 | 0.03 | 0.12 |
| (1,77) | 1:25:A:VAL:HG12 | 1:25:A:VAL:H | 4 | 0.14 | 0.03 | 0.12 |
| (1,77) | 1:25:A:VAL:HG13 | 1:25:A:VAL:H | 4 | 0.14 | 0.03 | 0.12 |
| (2,761) | 1:168:A:PHE:H | 1:169:A:ASP:H | 4 | 0.13 | 0.02 | 0.12 |
| (2,206) | 1:39:A:GLN:HB2 | 1:39:A:GLN:HE21 | 4 | 0.13 | 0.02 | 0.14 |
| (1,834) | 1:66:A:ASN:HB3 | 1:66:A:ASN:H | 4 | 0.12 | 0.01 | 0.13 |
| (1,2299) | 1:169:A:ASP:H | 1:170:A:SER:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,1380) | 1:87:A:THR:HA | 1:134:A:TRP:HH2 | 4 | 0.12 | 0.02 | 0.12 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG21 | 3 | 0.71 | 0.15 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG22 | 3 | 0.71 | 0.15 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG23 | 3 | 0.71 | 0.15 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG21 | 3 | 0.71 | 0.15 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG22 | 3 | 0.71 | 0.15 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG23 | 3 | 0.71 | 0.15 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG21 | 3 | 0.71 | 0.15 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG22 | 3 | 0.71 | 0.15 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG23 | 3 | 0.71 | 0.15 | 0.81 |
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE1 | 3 | 0.65 | 0.43 | 0.65 |
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE2 | 3 | 0.65 | 0.43 | 0.65 |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE1 | 3 | 0.65 | 0.43 | 0.65 |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE2 | 3 | 0.65 | 0.43 | 0.65 |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE1 | 3 | 0.65 | 0.43 | 0.65 |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE2 | 3 | 0.65 | 0.43 | 0.65 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD11 | 3 | 0.61 | 0.02 | 0.61 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD12 | 3 | 0.61 | 0.02 | 0.61 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD13 | 3 | 0.61 | 0.02 | 0.61 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,508) | 1:48:A:ILE:HG21 | 1:153:A:ILE:HG13 | 3 | 0.58 | 0.01 | 0.58 |
| (1,508) | 1:48:A:ILE:HG22 | 1:153:A:ILE:HG13 | 3 | 0.58 | 0.01 | 0.58 |
| (1,508) | 1:48:A:ILE:HG23 | 1:153:A:ILE:HG13 | 3 | 0.58 | 0.01 | 0.58 |
| (1,650) | 1:58:A:VAL:HG11 | 1:58:A:VAL:H | 3 | 0.58 | 0.03 | 0.6 |
| (1,650) | 1:58:A:VAL:HG12 | 1:58:A:VAL:H | 3 | 0.58 | 0.03 | 0.6 |
| (1,650) | 1:58:A:VAL:HG13 | 1:58:A:VAL:H | 3 | 0.58 | 0.03 | 0.6 |
| (1,650) | 1:58:A:VAL:HG21 | 1:58:A:VAL:H | 3 | 0.58 | 0.03 | 0.6 |
| (1,650) | 1:58:A:VAL:HG22 | 1:58:A:VAL:H | 3 | 0.58 | 0.03 | 0.6 |
| (1,650) | 1:58:A:VAL:HG23 | 1:58:A:VAL:H | 3 | 0.58 | 0.03 | 0.6 |
| (1,1274) | 1:82:A:THR:HG21 | 1:96:A:SER:HB3 | 3 | 0.58 | 0.02 | 0.58 |
| (1,1274) | 1:82:A:THR:HG22 | 1:96:A:SER:HB3 | 3 | 0.58 | 0.02 | 0.58 |
| (1,1274) | 1:82:A:THR:HG23 | 1:96:A:SER:HB3 | 3 | 0.58 | 0.02 | 0.58 |
| (1,1275) | 1:82:A:THR:HG21 | 1:96:A:SER:HB2 | 3 | 0.53 | 0.08 | 0.59 |
| (1,1275) | 1:82:A:THR:HG22 | 1:96:A:SER:HB2 | 3 | 0.53 | 0.08 | 0.59 |
| (1,1275) | 1:82:A:THR:HG23 | 1:96:A:SER:HB2 | 3 | 0.53 | 0.08 | 0.59 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD21 | 3 | 0.53 | 0.01 | 0.53 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD22 | 3 | 0.53 | 0.01 | 0.53 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD23 | 3 | 0.53 | 0.01 | 0.53 |
| (1,1766) | 1:120:A:VAL:HG11 | 1:120:A:VAL:H | 3 | 0.44 | 0.0 | 0.44 |
| (1,1766) | 1:120:A:VAL:HG12 | 1:120:A:VAL:H | 3 | 0.44 | 0.0 | 0.44 |
| (1,1766) | 1:120:A:VAL:HG13 | 1:120:A:VAL:H | 3 | 0.44 | 0.0 | 0.44 |
| (2,295) | 1:52:A:LYS:HE2 | 1:54:A:GLN:HE22 | 3 | 0.38 | 0.05 | 0.4 |
| (2,295) | 1:52:A:LYS:HE3 | 1:54:A:GLN:HE22 | 3 | 0.38 | 0.05 | 0.4 |
| (2,689) | 1:131:A:THR:HA | 1:145:A:TYR:HD1 | 3 | 0.37 | 0.09 | 0.44 |
| (2,689) | 1:131:A:THR:HA | 1:145:A:TYR:HD2 | 3 | 0.37 | 0.09 | 0.44 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD21 | 3 | 0.34 | 0.05 | 0.34 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD22 | 3 | 0.34 | 0.05 | 0.34 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD23 | 3 | 0.34 | 0.05 | 0.34 |
| (2,673) | 1:127:A:GLY:H | 1:128:A:TYR:HD1 | 3 | 0.33 | 0.12 | 0.25 |
| (2,673) | 1:127:A:GLY:H | 1:128:A:TYR:HD2 | 3 | 0.33 | 0.12 | 0.25 |
| (1,1557) | 1:103:A:SER:HA | 1:104:A:LEU:HB2 | 3 | 0.32 | 0.01 | 0.32 |
| (2,618) | 1:119:A:ALA:HB1 | 1:149:A:LYS:H | 3 | 0.31 | 0.18 | 0.21 |
| (2,618) | 1:119:A:ALA:HB2 | 1:149:A:LYS:H | 3 | 0.31 | 0.18 | 0.21 |
| (2,618) | 1:119:A:ALA:HB3 | 1:149:A:LYS:H | 3 | 0.31 | 0.18 | 0.21 |
| (1,1485) | 1:95:A:PHE:HE1 | 1:117:A:ASP:HA | 3 | 0.3 | 0.01 | 0.29 |
| (1,1485) | 1:95:A:PHE:HE2 | 1:117:A:ASP:HA | 3 | 0.3 | 0.01 | 0.29 |
| (1,2191) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HE1 | 3 | 0.29 | 0.11 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HE2 | 3 | 0.29 | 0.11 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HE1 | 3 | 0.29 | 0.11 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HE2 | 3 | 0.29 | 0.11 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HE1 | 3 | 0.29 | 0.11 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HE2 | 3 | 0.29 | 0.11 | 0.33 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1845) | 1:132:A:SER:HB2 | 1:145:A:TYR:HD1 | 3 | 0.28 | 0.04 | 0.3 |
| (1,1845) | 1:132:A:SER:HB2 | 1:145:A:TYR:HD2 | 3 | 0.28 | 0.04 | 0.3 |
| (1,2262) | 1:164:A:GLU:HA | 1:164:A:GLU:HG2 | 3 | 0.28 | 0.01 | 0.27 |
| (1,2262) | 1:164:A:GLU:HA | 1:164:A:GLU:HG3 | 3 | 0.28 | 0.01 | 0.27 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD11 | 3 | 0.27 | 0.08 | 0.23 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD12 | 3 | 0.27 | 0.08 | 0.23 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD13 | 3 | 0.27 | 0.08 | 0.23 |
| (1,1789) | 1:125:A:LYS:HG2 | 1:125:A:LYS:HE2 | 3 | 0.26 | 0.0 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG2 | 1:125:A:LYS:HE3 | 3 | 0.26 | 0.0 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG3 | 1:125:A:LYS:HE2 | 3 | 0.26 | 0.0 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG3 | 1:125:A:LYS:HE3 | 3 | 0.26 | 0.0 | 0.26 |
| (1,1770) | 1:120:A:VAL:HG21 | 1:121:A:LEU:H | 3 | 0.26 | 0.04 | 0.25 |
| (1,1770) | 1:120:A:VAL:HG22 | 1:121:A:LEU:H | 3 | 0.26 | 0.04 | 0.25 |
| (1,1770) | 1:120:A:VAL:HG23 | 1:121:A:LEU:H | 3 | 0.26 | 0.04 | 0.25 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG21 | 3 | 0.24 | 0.0 | 0.24 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG22 | 3 | 0.24 | 0.0 | 0.24 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG23 | 3 | 0.24 | 0.0 | 0.24 |
| (2,468) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HE1 | 3 | 0.24 | 0.02 | 0.25 |
| (2,468) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HE2 | 3 | 0.24 | 0.02 | 0.25 |
| (2,468) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HE1 | 3 | 0.24 | 0.02 | 0.25 |
| (2,468) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HE2 | 3 | 0.24 | 0.02 | 0.25 |
| (2,468) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HE1 | 3 | 0.24 | 0.02 | 0.25 |
| (2,468) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HE2 | 3 | 0.24 | 0.02 | 0.25 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB1 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB2 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB3 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB1 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB2 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB3 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB1 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB2 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB3 | 3 | 0.22 | 0.07 | 0.19 |
| (1,1474) | 1:95:A:PHE:HB2 | 1:95:A:PHE:H | 3 | 0.22 | 0.06 | 0.25 |
| (1,1474) | 1:95:A:PHE:HB3 | 1:95:A:PHE:H | 3 | 0.22 | 0.06 | 0.25 |
| (1,1635) | 1:111:A:ILE:HB | 1:111:A:ILE:H | 3 | 0.21 | 0.02 | 0.21 |
| (1,1020) | 1:74:A:PHE:HD1 | 1:162:A:ALA:HA | 3 | 0.2 | 0.08 | 0.22 |
| (1,1020) | 1:74:A:PHE:HD2 | 1:162:A:ALA:HA | 3 | 0.2 | 0.08 | 0.22 |
| (1,647) | 1:58:A:VAL:HB | 1:58:A:VAL:H | 3 | 0.2 | 0.0 | 0.2 |
| (1,2425) | 1:177:A:PHE:HD1 | 1:177:A:PHE:H | 3 | 0.19 | 0.06 | 0.22 |
| (1,2425) | 1:177:A:PHE:HD2 | 1:177:A:PHE:H | 3 | 0.19 | 0.06 | 0.22 |
| (1,1232) | 1:81:A:ILE:HG21 | 1:99:A:LYS:H | 3 | 0.19 | 0.08 | 0.16 |
| (1,1232) | 1:81:A:ILE:HG22 | 1:99:A:LYS:H | 3 | 0.19 | 0.08 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1232) | 1:81:A:ILE:HG23 | 1:99:A:LYS:H | 3 | 0.19 | 0.08 | 0.16 |
| (1,356) | 1:42:A:ASP:HB2 | 1:160:A:TYR:HE1 | 3 | 0.19 | 0.12 | 0.11 |
| (1,356) | 1:42:A:ASP:HB2 | 1:160:A:TYR:HE2 | 3 | 0.19 | 0.12 | 0.11 |
| (1,356) | 1:42:A:ASP:HB3 | 1:160:A:TYR:HE1 | 3 | 0.19 | 0.12 | 0.11 |
| (1,356) | 1:42:A:ASP:HB3 | 1:160:A:TYR:HE2 | 3 | 0.19 | 0.12 | 0.11 |
| (1,1882) | 1:134:A:TRP:HA | 1:143:A:ILE:HA | 3 | 0.18 | 0.01 | 0.19 |
| (1,1775) | 1:121:A:LEU:HB2 | 1:121:A:LEU:H | 3 | 0.18 | 0.03 | 0.19 |
| (1,1572) | 1:104:A:LEU:HD11 | 1:104:A:LEU:H | 3 | 0.17 | 0.02 | 0.17 |
| (1,1572) | 1:104:A:LEU:HD12 | 1:104:A:LEU:H | 3 | 0.17 | 0.02 | 0.17 |
| (1,1572) | 1:104:A:LEU:HD13 | 1:104:A:LEU:H | 3 | 0.17 | 0.02 | 0.17 |
| (1,886) | 1:68:A:GLU:HA | 1:71:A:LYS:HD2 | 3 | 0.16 | 0.06 | 0.14 |
| (1,886) | 1:68:A:GLU:HA | 1:71:A:LYS:HD3 | 3 | 0.16 | 0.06 | 0.14 |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE1 | 3 | 0.16 | 0.06 | 0.13 |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE2 | 3 | 0.16 | 0.06 | 0.13 |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE1 | 3 | 0.16 | 0.06 | 0.13 |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE2 | 3 | 0.16 | 0.06 | 0.13 |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE1 | 3 | 0.16 | 0.06 | 0.13 |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE2 | 3 | 0.16 | 0.06 | 0.13 |
| (2,298) | 1:54:A:GLN:HB3 | 1:54:A:GLN:HE21 | 3 | 0.16 | 0.03 | 0.14 |
| (3,2) | 1:33:A:THR:HA | 1:34:A:PRO:HD3 | 3 | 0.16 | 0.03 | 0.15 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD11 | 3 | 0.15 | 0.03 | 0.17 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD12 | 3 | 0.15 | 0.03 | 0.17 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD13 | 3 | 0.15 | 0.03 | 0.17 |
| (1,2316) | 1:171:A:LEU:HA | 1:172:A:PRO:HD3 | 3 | 0.15 | 0.03 | 0.16 |
| (1,256) | 1:33:A:THR:HA | 1:168:A:PHE:HZ | 3 | 0.14 | 0.03 | 0.14 |
| (1,12) | 1:21:A:GLU:HA | 1:21:A:GLU:HG2 | 3 | 0.13 | 0.0 | 0.13 |
| (1,12) | 1:21:A:GLU:HA | 1:21:A:GLU:HG3 | 3 | 0.13 | 0.0 | 0.13 |
| (1,424) | 1:46:A:TYR:HA | 1:155:A:ASN:HB2 | 3 | 0.12 | 0.01 | 0.12 |
| (1,272) | 1:34:A:PRO:HD2 | 1:35:A:ALA:H | 3 | 0.11 | 0.01 | 0.12 |
| (1,432) | 1:46:A:TYR:HB3 | 1:154:A:LEU:H | 3 | 0.11 | 0.01 | 0.11 |
| (1,1422) | 1:88:A:ASN:HB2 | 1:88:A:ASN:HD21 | 3 | 0.11 | 0.01 | 0.12 |
| (1,1629) | 1:110:A:VAL:HG11 | 1:111:A:ILE:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,1629) | 1:110:A:VAL:HG12 | 1:111:A:ILE:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,1629) | 1:110:A:VAL:HG13 | 1:111:A:ILE:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB1 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB3 | 3 | 0.11 | 0.0 | 0.11 |
| (1,678) | 1:60:A:LEU:HA | 1:111:A:ILE:H | 3 | 0.1 | 0.0 | 0.1 |
| (1,1457) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 2 | 0.72 | 0.03 | 0.72 |
| (1,1457) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 2 | 0.72 | 0.03 | 0.72 |
| (1,1457) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 2 | 0.72 | 0.03 | 0.72 |
| (2,5) | 1:16:A:ALA:HB1 | 1:17:A:GLN:HE21 | 2 | 0.65 | 0.1 | 0.65 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,5) | 1:16:A:ALA:HB2 | 1:17:A:GLN:HE21 | 2 | 0.65 | 0.1 | 0.65 |
| (2,5) | 1:16:A:ALA:HB3 | 1:17:A:GLN:HE21 | 2 | 0.65 | 0.1 | 0.65 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB1 | 2 | 0.65 | 0.03 | 0.65 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB2 | 2 | 0.65 | 0.03 | 0.65 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB3 | 2 | 0.65 | 0.03 | 0.65 |
| (1,1091) | 1:77:A:LEU:HD11 | 1:103:A:SER:HA | 2 | 0.53 | 0.14 | 0.53 |
| (1,1091) | 1:77:A:LEU:HD12 | 1:103:A:SER:HA | 2 | 0.53 | 0.14 | 0.53 |
| (1,1091) | 1:77:A:LEU:HD13 | 1:103:A:SER:HA | 2 | 0.53 | 0.14 | 0.53 |
| (1,1091) | 1:77:A:LEU:HD21 | 1:103:A:SER:HA | 2 | 0.53 | 0.14 | 0.53 |
| (1,1091) | 1:77:A:LEU:HD22 | 1:103:A:SER:HA | 2 | 0.53 | 0.14 | 0.53 |
| (1,1091) | 1:77:A:LEU:HD23 | 1:103:A:SER:HA | 2 | 0.53 | 0.14 | 0.53 |
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE1 | 2 | 0.52 | 0.26 | 0.52 |
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE2 | 2 | 0.52 | 0.26 | 0.52 |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE1 | 2 | 0.52 | 0.26 | 0.52 |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE2 | 2 | 0.52 | 0.26 | 0.52 |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE1 | 2 | 0.52 | 0.26 | 0.52 |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE2 | 2 | 0.52 | 0.26 | 0.52 |
| (2,700) | 1:132:A:SER:HB3 | 1:145:A:TYR:HE1 | 2 | 0.51 | 0.0 | 0.51 |
| (2,700) | 1:132:A:SER:HB3 | 1:145:A:TYR:HE2 | 2 | 0.51 | 0.0 | 0.51 |
| (2,716) | 1:142:A:ILE:HB | 1:145:A:TYR:HE1 | 2 | 0.51 | 0.0 | 0.51 |
| (2,716) | 1:142:A:ILE:HB | 1:145:A:TYR:HE2 | 2 | 0.51 | 0.0 | 0.51 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD11 | 2 | 0.49 | 0.09 | 0.49 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD12 | 2 | 0.49 | 0.09 | 0.49 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD13 | 2 | 0.49 | 0.09 | 0.49 |
| (1,1662) | 1:113:A:LEU:HD11 | 1:113:A:LEU:H | 2 | 0.48 | 0.0 | 0.48 |
| (1,1662) | 1:113:A:LEU:HD12 | 1:113:A:LEU:H | 2 | 0.48 | 0.0 | 0.48 |
| (1,1662) | 1:113:A:LEU:HD13 | 1:113:A:LEU:H | 2 | 0.48 | 0.0 | 0.48 |
| (2,661) | 1:125:A:LYS:HG2 | 1:126:A:THR:H | 2 | 0.46 | 0.06 | 0.46 |
| (2,661) | 1:125:A:LYS:HG3 | 1:126:A:THR:H | 2 | 0.46 | 0.06 | 0.46 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD21 | 2 | 0.44 | 0.25 | 0.44 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD22 | 2 | 0.44 | 0.25 | 0.44 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD23 | 2 | 0.44 | 0.25 | 0.44 |
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD21 | 2 | 0.44 | 0.25 | 0.44 |
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD22 | 2 | 0.44 | 0.25 | 0.44 |
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD23 | 2 | 0.44 | 0.25 | 0.44 |
| (1,2081) | 1:151:A:VAL:HG11 | 1:153:A:ILE:H | 2 | 0.44 | 0.03 | 0.44 |
| (1,2081) | 1:151:A:VAL:HG12 | 1:153:A:ILE:H | 2 | 0.44 | 0.03 | 0.44 |
| (1,2081) | 1:151:A:VAL:HG13 | 1:153:A:ILE:H | 2 | 0.44 | 0.03 | 0.44 |
| (2,240) | 1:46:A:TYR:HB2 | 1:155:A:ASN:HD21 | 2 | 0.44 | 0.03 | 0.44 |
| (2,240) | 1:46:A:TYR:HB2 | 1:155:A:ASN:HD22 | 2 | 0.44 | 0.03 | 0.44 |
| (1,2080) | 1:151:A:VAL:HG11 | 1:152:A:ALA:H | 2 | 0.42 | 0.01 | 0.42 |
| (1,2080) | 1:151:A:VAL:HG12 | 1:152:A:ALA:H | 2 | 0.42 | 0.01 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2080) | 1:151:A:VAL:HG13 | 1:152:A:ALA:H | 2 | 0.42 | 0.01 | 0.42 |
| (2,355) | 1:64:A:LEU:H | 1:175:A:PHE:HE1 | 2 | 0.4 | 0.1 | 0.4 |
| (2,355) | 1:64:A:LEU:H | 1:175:A:PHE:HE2 | 2 | 0.4 | 0.1 | 0.4 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG21 | 2 | 0.4 | 0.05 | 0.4 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG22 | 2 | 0.4 | 0.05 | 0.4 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG23 | 2 | 0.4 | 0.05 | 0.4 |
| (1,2287) | 1:168:A:PHE:HD1 | 1:169:A:ASP:H | 2 | 0.38 | 0.21 | 0.38 |
| (1,2287) | 1:168:A:PHE:HD2 | 1:169:A:ASP:H | 2 | 0.38 | 0.21 | 0.38 |
| (2,721) | 1:144:A:VAL:HA | 1:145:A:TYR:HD1 | 2 | 0.37 | 0.2 | 0.37 |
| (2,721) | 1:144:A:VAL:HA | 1:145:A:TYR:HD2 | 2 | 0.37 | 0.2 | 0.37 |
| (1,126) | 1:27:A:SER:HB2 | 1:177:A:PHE:HE1 | 2 | 0.36 | 0.12 | 0.36 |
| (1,126) | 1:27:A:SER:HB2 | 1:177:A:PHE:HE2 | 2 | 0.36 | 0.12 | 0.36 |
| (1,126) | 1:27:A:SER:HB3 | 1:177:A:PHE:HE1 | 2 | 0.36 | 0.12 | 0.36 |
| (1,126) | 1:27:A:SER:HB3 | 1:177:A:PHE:HE2 | 2 | 0.36 | 0.12 | 0.36 |
| (2,601) | 1:115:A:LYS:HE2 | 1:116:A:GLU:H | 2 | 0.36 | 0.04 | 0.36 |
| (2,601) | 1:115:A:LYS:HE3 | 1:116:A:GLU:H | 2 | 0.36 | 0.04 | 0.36 |
| (2,725) | 1:145:A:TYR:HD1 | 1:147:A:GLU:H | 2 | 0.36 | 0.01 | 0.36 |
| (2,725) | 1:145:A:TYR:HD2 | 1:147:A:GLU:H | 2 | 0.36 | 0.01 | 0.36 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD11 | 2 | 0.36 | 0.14 | 0.36 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD12 | 2 | 0.36 | 0.14 | 0.36 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD13 | 2 | 0.36 | 0.14 | 0.36 |
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG21 | 2 | 0.34 | 0.1 | 0.34 |
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG22 | 2 | 0.34 | 0.1 | 0.34 |
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG23 | 2 | 0.34 | 0.1 | 0.34 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG21 | 2 | 0.34 | 0.1 | 0.34 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG22 | 2 | 0.34 | 0.1 | 0.34 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG23 | 2 | 0.34 | 0.1 | 0.34 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG21 | 2 | 0.34 | 0.1 | 0.34 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG22 | 2 | 0.34 | 0.1 | 0.34 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG23 | 2 | 0.34 | 0.1 | 0.34 |
| (1,2069) | 1:148:A:THR:HG21 | 1:148:A:THR:H | 2 | 0.34 | 0.2 | 0.34 |
| (1,2069) | 1:148:A:THR:HG22 | 1:148:A:THR:H | 2 | 0.34 | 0.2 | 0.34 |
| (1,2069) | 1:148:A:THR:HG23 | 1:148:A:THR:H | 2 | 0.34 | 0.2 | 0.34 |
| (2,724) | 1:145:A:TYR:HD1 | 1:147:A:GLU:HG2 | 2 | 0.34 | 0.04 | 0.34 |
| (2,724) | 1:145:A:TYR:HD1 | 1:147:A:GLU:HG3 | 2 | 0.34 | 0.04 | 0.34 |
| (2,724) | 1:145:A:TYR:HD2 | 1:147:A:GLU:HG2 | 2 | 0.34 | 0.04 | 0.34 |
| (2,724) | 1:145:A:TYR:HD2 | 1:147:A:GLU:HG3 | 2 | 0.34 | 0.04 | 0.34 |
| (1,238) | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB2 | 2 | 0.32 | 0.01 | 0.32 |
| (1,238) | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB3 | 2 | 0.32 | 0.01 | 0.32 |
| (1,238) | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB2 | 2 | 0.32 | 0.01 | 0.32 |
| (1,238) | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB3 | 2 | 0.32 | 0.01 | 0.32 |
| (1,238) | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB2 | 2 | 0.32 | 0.01 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,238) | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB3 | 2 | 0.32 | 0.01 | 0.32 |
| (2,443) | 1:76:A:TYR:HE1 | 1:78:A:GLN:HE22 | 2 | 0.32 | 0.2 | 0.32 |
| (2,443) | 1:76:A:TYR:HE2 | 1:78:A:GLN:HE22 | 2 | 0.32 | 0.2 | 0.32 |
| (1,2176) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HE1 | 2 | 0.32 | 0.15 | 0.32 |
| (1,2176) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HE2 | 2 | 0.32 | 0.15 | 0.32 |
| (1,2176) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HE1 | 2 | 0.32 | 0.15 | 0.32 |
| (1,2176) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HE2 | 2 | 0.32 | 0.15 | 0.32 |
| (1,2446) | 1:179:A:VAL:HB | 1:179:A:VAL:H | 2 | 0.32 | 0.01 | 0.32 |
| (2,227) | 1:43:A:ASP:HB3 | 1:46:A:TYR:HE1 | 2 | 0.32 | 0.08 | 0.32 |
| (2,227) | 1:43:A:ASP:HB3 | 1:46:A:TYR:HE2 | 2 | 0.32 | 0.08 | 0.32 |
| (1,1460) | 1:92:A:LEU:HG | 1:93:A:GLY:H | 2 | 0.31 | 0.16 | 0.31 |
| (1,1841) | 1:132:A:SER:HB3 | 1:145:A:TYR:HD1 | 2 | 0.3 | 0.01 | 0.3 |
| (1,1841) | 1:132:A:SER:HB3 | 1:145:A:TYR:HD2 | 2 | 0.3 | 0.01 | 0.3 |
| (1,260) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD3 | 2 | 0.29 | 0.1 | 0.29 |
| (1,260) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD3 | 2 | 0.29 | 0.1 | 0.29 |
| (1,260) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD3 | 2 | 0.29 | 0.1 | 0.29 |
| (1,2321) | 1:171:A:LEU:HD11 | 1:171:A:LEU:H | 2 | 0.29 | 0.06 | 0.29 |
| (1,2321) | 1:171:A:LEU:HD12 | 1:171:A:LEU:H | 2 | 0.29 | 0.06 | 0.29 |
| (1,2321) | 1:171:A:LEU:HD13 | 1:171:A:LEU:H | 2 | 0.29 | 0.06 | 0.29 |
| (1,1032) | 1:74:A:PHE:HE1 | 1:168:A:PHE:HZ | 2 | 0.28 | 0.03 | 0.28 |
| (1,1032) | 1:74:A:PHE:HE2 | 1:168:A:PHE:HZ | 2 | 0.28 | 0.03 | 0.28 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD11 | 2 | 0.27 | 0.1 | 0.27 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD12 | 2 | 0.27 | 0.1 | 0.27 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD13 | 2 | 0.27 | 0.1 | 0.27 |
| (1,724) | 1:62:A:VAL:HG11 | 1:63:A:THR:H | 2 | 0.27 | 0.01 | 0.27 |
| (1,724) | 1:62:A:VAL:HG12 | 1:63:A:THR:H | 2 | 0.27 | 0.01 | 0.27 |
| (1,724) | 1:62:A:VAL:HG13 | 1:63:A:THR:H | 2 | 0.27 | 0.01 | 0.27 |
| (1,1400) | 1:87:A:THR:HG21 | 1:88:A:ASN:HA | 2 | 0.27 | 0.05 | 0.27 |
| (1,1400) | 1:87:A:THR:HG22 | 1:88:A:ASN:HA | 2 | 0.27 | 0.05 | 0.27 |
| (1,1400) | 1:87:A:THR:HG23 | 1:88:A:ASN:HA | 2 | 0.27 | 0.05 | 0.27 |
| (2,522) | 1:85:A:TYR:HD1 | 1:134:A:TRP:HA | 2 | 0.27 | 0.01 | 0.27 |
| (2,522) | 1:85:A:TYR:HD2 | 1:134:A:TRP:HA | 2 | 0.27 | 0.01 | 0.27 |
| (1,651) | 1:58:A:VAL:HG11 | 1:59:A:LYS:H | 2 | 0.26 | 0.11 | 0.26 |
| (1,651) | 1:58:A:VAL:HG12 | 1:59:A:LYS:H | 2 | 0.26 | 0.11 | 0.26 |
| (1,651) | 1:58:A:VAL:HG13 | 1:59:A:LYS:H | 2 | 0.26 | 0.11 | 0.26 |
| (1,651) | 1:58:A:VAL:HG21 | 1:59:A:LYS:H | 2 | 0.26 | 0.11 | 0.26 |
| (1,651) | 1:58:A:VAL:HG22 | 1:59:A:LYS:H | 2 | 0.26 | 0.11 | 0.26 |
| (1,651) | 1:58:A:VAL:HG23 | 1:59:A:LYS:H | 2 | 0.26 | 0.11 | 0.26 |
| (1,727) | 1:62:A:VAL:HG11 | 1:177:A:PHE:HE1 | 2 | 0.26 | 0.02 | 0.26 |
| (1,727) | 1:62:A:VAL:HG11 | 1:177:A:PHE:HE2 | 2 | 0.26 | 0.02 | 0.26 |
| (1,727) | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE1 | 2 | 0.26 | 0.02 | 0.26 |
| (1,727) | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE2 | 2 | 0.26 | 0.02 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,727) | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE1 | 2 | 0.26 | 0.02 | 0.26 |
| (1,727) | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE2 | 2 | 0.26 | 0.02 | 0.26 |
| (2,547) | 1:87:A:THR:HG21 | 1:91:A:ALA:H | 2 | 0.26 | 0.03 | 0.26 |
| (2,547) | 1:87:A:THR:HG22 | 1:91:A:ALA:H | 2 | 0.26 | 0.03 | 0.26 |
| (2,547) | 1:87:A:THR:HG23 | 1:91:A:ALA:H | 2 | 0.26 | 0.03 | 0.26 |
| (1,445) | 1:46:A:TYR:HE1 | 1:141:A:LYS:HE3 | 2 | 0.25 | 0.06 | 0.25 |
| (1,445) | 1:46:A:TYR:HE2 | 1:141:A:LYS:HE3 | 2 | 0.25 | 0.06 | 0.25 |
| (1,728) | 1:62:A:VAL:HG21 | 1:62:A:VAL:H | 2 | 0.23 | 0.01 | 0.23 |
| (1,728) | 1:62:A:VAL:HG22 | 1:62:A:VAL:H | 2 | 0.23 | 0.01 | 0.23 |
| (1,728) | 1:62:A:VAL:HG23 | 1:62:A:VAL:H | 2 | 0.23 | 0.01 | 0.23 |
| (2,552) | 1:87:A:THR:H | 1:92:A:LEU:HB2 | 2 | 0.23 | 0.02 | 0.23 |
| (1,392) | 1:44:A:ILE:HG21 | 1:158:A:ALA:H | 2 | 0.22 | 0.02 | 0.22 |
| (1,392) | 1:44:A:ILE:HG22 | 1:158:A:ALA:H | 2 | 0.22 | 0.02 | 0.22 |
| (1,392) | 1:44:A:ILE:HG23 | 1:158:A:ALA:H | 2 | 0.22 | 0.02 | 0.22 |
| (1,941) | 1:71:A:LYS:HA | 1:74:A:PHE:HD1 | 2 | 0.22 | 0.02 | 0.22 |
| (1,941) | 1:71:A:LYS:HA | 1:74:A:PHE:HD2 | 2 | 0.22 | 0.02 | 0.22 |
| (1,498) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HZ2 | 2 | 0.2 | 0.03 | 0.2 |
| (1,498) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HZ2 | 2 | 0.2 | 0.03 | 0.2 |
| (1,498) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HZ2 | 2 | 0.2 | 0.03 | 0.2 |
| (2,625) | 1:121:A:LEU:H | 1:122:A:TYR:HD1 | 2 | 0.2 | 0.08 | 0.2 |
| (2,625) | 1:121:A:LEU:H | 1:122:A:TYR:HD2 | 2 | 0.2 | 0.08 | 0.2 |
| (1,1793) | 1:128:A:TYR:HA | 1:128:A:TYR:HB3 | 2 | 0.2 | 0.05 | 0.2 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG21 | 2 | 0.18 | 0.04 | 0.18 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG22 | 2 | 0.18 | 0.04 | 0.18 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG23 | 2 | 0.18 | 0.04 | 0.18 |
| (1,912) | 1:69:A:GLN:HG3 | 1:69:A:GLN:HE21 | 2 | 0.18 | 0.03 | 0.18 |
| (1,46) | 1:24:A:ASP:HB3 | 1:50:A:TRP:HB3 | 2 | 0.18 | 0.0 | 0.18 |
| (1,1446) | 1:90:A:THR:HA | 1:93:A:GLY:H | 2 | 0.18 | 0.04 | 0.18 |
| (1,2272) | 1:166:A:MET:HB2 | 1:167:A:LEU:H | 2 | 0.18 | 0.0 | 0.18 |
| (1,530) | 1:49:A:VAL:H | 1:152:A:ALA:HA | 2 | 0.17 | 0.0 | 0.17 |
| (1,989) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HE1 | 2 | 0.17 | 0.02 | 0.17 |
| (1,989) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HE2 | 2 | 0.17 | 0.02 | 0.17 |
| (1,989) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HE1 | 2 | 0.17 | 0.02 | 0.17 |
| (1,989) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HE2 | 2 | 0.17 | 0.02 | 0.17 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (2,760) | 1:168:A:PHE:HE1 | 1:171:A:LEU:HG | 2 | 0.16 | 0.02 | 0.16 |
| (2,760) | 1:168:A:PHE:HE2 | 1:171:A:LEU:HG | 2 | 0.16 | 0.02 | 0.16 |
| (1,337) | 1:41:A:SER:HB2 | 1:42:A:ASP:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1272) | 1:82:A:THR:HG21 | 1:96:A:SER:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1272) | 1:82:A:THR:HG22 | 1:96:A:SER:HA | 2 | 0.14 | 0.0 | 0.14 |

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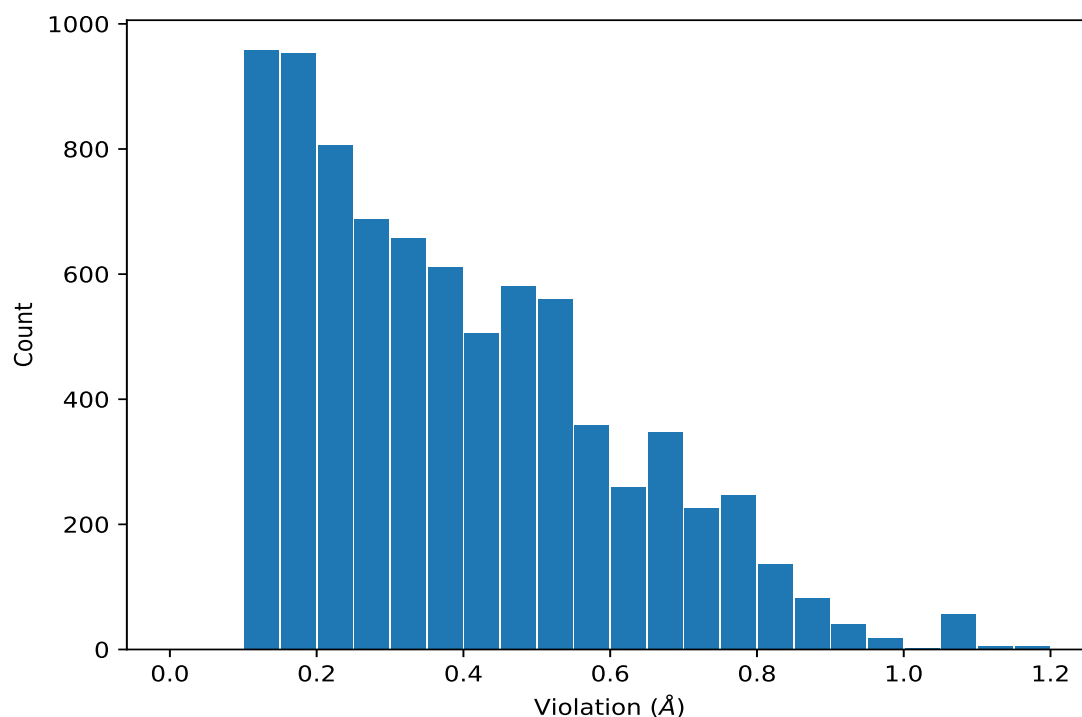
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1272) | 1:82:A:THR:HG23 | 1:96:A:SER:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1273) | 1:82:A:THR:HG21 | 1:96:A:SER:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1273) | 1:82:A:THR:HG22 | 1:96:A:SER:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1273) | 1:82:A:THR:HG23 | 1:96:A:SER:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1335) | 1:85:A:TYR:HB2 | 1:86:A:GLU:H | 2 | 0.14 | 0.0 | 0.14 |
| (1,2276) | 1:167:A:LEU:H | 1:168:A:PHE:H | 2 | 0.14 | 0.03 | 0.14 |
| (2,12) | 1:17:A:GLN:HB2 | 1:17:A:GLN:HE21 | 2 | 0.14 | 0.0 | 0.14 |
| (1,259) | 1:33:A:THR:HB | 1:35:A:ALA:H | 2 | 0.13 | 0.0 | 0.13 |
| (1,863) | 1:66:A:ASN:H | 1:175:A:PHE:HA | 2 | 0.13 | 0.01 | 0.13 |
| (1,1100) | 1:77:A:LEU:HG | 1:78:A:GLN:H | 2 | 0.13 | 0.02 | 0.13 |
| (1,54) | 1:24:A:ASP:HB2 | 1:50:A:TRP:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,447) | 1:46:A:TYR:HE1 | 1:141:A:LYS:HG3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,447) | 1:46:A:TYR:HE2 | 1:141:A:LYS:HG3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,529) | 1:49:A:VAL:H | 1:151:A:VAL:HA | 2 | 0.12 | 0.02 | 0.12 |
| (1,1333) | 1:85:A:TYR:HA | 1:86:A:GLU:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1086) | 1:77:A:LEU:HB2 | 1:78:A:GLN:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,1282) | 1:82:A:THR:H | 1:155:A:ASN:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1690) | 1:115:A:LYS:HA | 1:115:A:LYS:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1690) | 1:115:A:LYS:HA | 1:115:A:LYS:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1817) | 1:131:A:THR:HB | 1:132:A:SER:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,2271) | 1:166:A:MET:HB3 | 1:167:A:LEU:H | 2 | 0.12 | 0.01 | 0.12 |
| (2,26) | 1:19:A:VAL:H | 1:20:A:SER:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,26) | 1:19:A:VAL:H | 1:20:A:SER:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1439) | 1:88:A:ASN:H | 1:134:A:TRP:HZ3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1271) | 1:82:A:THR:HG21 | 1:83:A:SER:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,1271) | 1:82:A:THR:HG22 | 1:83:A:SER:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,1271) | 1:82:A:THR:HG23 | 1:83:A:SER:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,188) | 1:30:A:GLY:H | 1:46:A:TYR:H | 2 | 0.11 | 0.0 | 0.11 |
| (2,27) | 1:19:A:VAL:H | 1:20:A:SER:H | 2 | 0.11 | 0.01 | 0.11 |
| (2,123) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 2 | 0.11 | 0.0 | 0.11 |
| (2,123) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,141) | 1:28:A:HIS:HD2 | 1:48:A:ILE:HA | 2 | 0.11 | 0.0 | 0.11 |
| (1,290) | 1:37:A:GLY:HA3 | 1:38:A:ALA:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,639) | 1:57:A:ASP:HB3 | 1:58:A:VAL:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,828) | 1:66:A:ASN:HA | 1:69:A:GLN:HG3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1761) | 1:119:A:ALA:H | 1:151:A:VAL:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,2295) | 1:169:A:ASP:HB3 | 1:170:A:SER:H | 2 | 0.11 | 0.0 | 0.11 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE1 | 6 | 1.18 |
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE2 | 6 | 1.18 |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE1 | 6 | 1.18 |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE2 | 6 | 1.18 |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE1 | 6 | 1.18 |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE2 | 6 | 1.18 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 5 | 1.11 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 5 | 1.11 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 5 | 1.11 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 5 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 5 | 1.11 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 5 | 1.11 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 4 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 4 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 4 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 4 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 4 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 4 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 9 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 9 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 9 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 9 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 9 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 9 | 1.08 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 1 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 1 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 1 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 1 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 1 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 1 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 7 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 7 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 7 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 7 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 7 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 7 | 1.07 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 7 | 1.07 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 7 | 1.07 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 7 | 1.07 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 4 | 1.07 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 4 | 1.07 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 4 | 1.07 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 4 | 1.07 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 4 | 1.07 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 4 | 1.07 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 5 | 1.06 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 5 | 1.06 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 5 | 1.06 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 5 | 1.06 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 5 | 1.06 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 5 | 1.06 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 8 | 1.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 8 | 1.06 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 8 | 1.06 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 8 | 1.06 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 8 | 1.06 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 8 | 1.06 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 9 | 1.06 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 9 | 1.06 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 9 | 1.06 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 9 | 1.06 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 9 | 1.06 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 9 | 1.06 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 7 | 1.05 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 7 | 1.05 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 7 | 1.05 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 7 | 1.05 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 7 | 1.05 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 7 | 1.05 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD11 | 2 | 1.01 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD12 | 2 | 1.01 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD13 | 2 | 1.01 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 3 | 0.98 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 3 | 0.98 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 3 | 0.98 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 3 | 0.98 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 3 | 0.98 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 3 | 0.98 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB2 | 7 | 0.97 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB3 | 7 | 0.97 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB2 | 7 | 0.97 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB3 | 7 | 0.97 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB2 | 7 | 0.97 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB3 | 7 | 0.97 |
| (1,2017) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HE1 | 6 | 0.96 |
| (1,2017) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HE2 | 6 | 0.96 |
| (1,2017) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HE1 | 6 | 0.96 |
| (1,2017) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HE2 | 6 | 0.96 |
| (1,2017) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HE1 | 6 | 0.96 |
| (1,2017) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HE2 | 6 | 0.96 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 4 | 0.94 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 4 | 0.94 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 4 | 0.94 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 4 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 3 | 0.93 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 3 | 0.93 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 3 | 0.93 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 3 | 0.93 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 9 | 0.93 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 9 | 0.93 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 9 | 0.93 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 9 | 0.93 |
| (2,437) | 1:76:A:TYR:HD1 | 1:104:A:LEU:HD11 | 10 | 0.93 |
| (2,437) | 1:76:A:TYR:HD1 | 1:104:A:LEU:HD12 | 10 | 0.93 |
| (2,437) | 1:76:A:TYR:HD1 | 1:104:A:LEU:HD13 | 10 | 0.93 |
| (2,437) | 1:76:A:TYR:HD2 | 1:104:A:LEU:HD11 | 10 | 0.93 |
| (2,437) | 1:76:A:TYR:HD2 | 1:104:A:LEU:HD12 | 10 | 0.93 |
| (2,437) | 1:76:A:TYR:HD2 | 1:104:A:LEU:HD13 | 10 | 0.93 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 6 | 0.93 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 6 | 0.93 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 6 | 0.93 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 6 | 0.93 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 6 | 0.93 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 6 | 0.93 |
| (1,21) | 1:22:A:PRO:HD2 | 1:23:A:ILE:H | 3 | 0.93 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 6 | 0.92 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 6 | 0.92 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 6 | 0.92 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 10 | 0.91 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 10 | 0.91 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 10 | 0.91 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 10 | 0.91 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 10 | 0.91 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 10 | 0.91 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 5 | 0.9 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 5 | 0.9 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 5 | 0.9 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 5 | 0.9 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 5 | 0.9 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 5 | 0.9 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 10 | 0.89 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 10 | 0.89 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 10 | 0.89 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 10 | 0.89 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 1 | 0.89 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 1 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 1 | 0.89 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 9 | 0.89 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 9 | 0.89 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 9 | 0.89 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 1 | 0.89 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 1 | 0.89 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 1 | 0.89 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 1 | 0.89 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 1 | 0.89 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 1 | 0.89 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 2 | 0.88 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 2 | 0.88 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 2 | 0.88 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 4 | 0.88 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 4 | 0.88 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 4 | 0.88 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 5 | 0.88 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 5 | 0.88 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 5 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 8 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 8 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 8 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 8 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 8 | 0.88 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 8 | 0.88 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 8 | 0.88 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 8 | 0.88 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 8 | 0.88 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 8 | 0.88 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 8 | 0.88 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 8 | 0.88 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 7 | 0.87 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 7 | 0.87 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 7 | 0.87 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 4 | 0.87 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 4 | 0.87 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 4 | 0.87 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 9 | 0.87 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 9 | 0.87 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 9 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 3 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 3 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 3 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 3 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 3 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 3 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 4 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 4 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 4 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 4 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 4 | 0.87 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 4 | 0.87 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB2 | 4 | 0.87 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB3 | 4 | 0.87 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB2 | 4 | 0.87 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB3 | 4 | 0.87 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB2 | 4 | 0.87 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB3 | 4 | 0.87 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 3 | 0.86 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 3 | 0.86 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 3 | 0.86 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 7 | 0.86 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 7 | 0.86 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 7 | 0.86 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 7 | 0.86 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 7 | 0.86 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 7 | 0.86 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 8 | 0.85 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 8 | 0.85 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 8 | 0.85 |
| (2,469) | 1:79:A:ILE:HG21 | 1:157:A:LYS:H | 10 | 0.85 |
| (2,469) | 1:79:A:ILE:HG22 | 1:157:A:LYS:H | 10 | 0.85 |
| (2,469) | 1:79:A:ILE:HG23 | 1:157:A:LYS:H | 10 | 0.85 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 10 | 0.85 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 10 | 0.85 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 10 | 0.85 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 8 | 0.84 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 8 | 0.84 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 8 | 0.84 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 8 | 0.84 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 1 | 0.84 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 1 | 0.84 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 1 | 0.84 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 7 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 7 | 0.84 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 7 | 0.84 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 3 | 0.84 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 3 | 0.84 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 3 | 0.84 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 9 | 0.84 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 9 | 0.84 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 9 | 0.84 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 10 | 0.83 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 10 | 0.83 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 10 | 0.83 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 10 | 0.83 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 10 | 0.83 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 10 | 0.83 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 4 | 0.82 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 4 | 0.82 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 4 | 0.82 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 8 | 0.82 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 8 | 0.82 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 8 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG21 | 7 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG22 | 7 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG23 | 7 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG21 | 7 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG22 | 7 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG23 | 7 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG21 | 7 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG22 | 7 | 0.82 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG23 | 7 | 0.82 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 10 | 0.82 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 10 | 0.82 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 10 | 0.82 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 10 | 0.82 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 10 | 0.82 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 10 | 0.82 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 3 | 0.81 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 3 | 0.81 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 3 | 0.81 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 2 | 0.81 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 2 | 0.81 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 2 | 0.81 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 5 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 5 | 0.81 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 5 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG21 | 6 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG22 | 6 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG23 | 6 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG21 | 6 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG22 | 6 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG23 | 6 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG21 | 6 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG22 | 6 | 0.81 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG23 | 6 | 0.81 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 2 | 0.81 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 2 | 0.81 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 2 | 0.81 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 8 | 0.81 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 8 | 0.81 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 8 | 0.81 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 10 | 0.8 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 10 | 0.8 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 10 | 0.8 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 10 | 0.8 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 1 | 0.8 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 1 | 0.8 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 1 | 0.8 |
| (2,386) | 1:70:A:LEU:HD11 | 1:172:A:PRO:HD2 | 9 | 0.8 |
| (2,386) | 1:70:A:LEU:HD12 | 1:172:A:PRO:HD2 | 9 | 0.8 |
| (2,386) | 1:70:A:LEU:HD13 | 1:172:A:PRO:HD2 | 9 | 0.8 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 1 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 1 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 1 | 0.8 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 2 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 2 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 2 | 0.8 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 3 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 3 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 3 | 0.8 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 5 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 5 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 5 | 0.8 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 6 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 6 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 6 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 7 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 7 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 7 | 0.8 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 8 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 8 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 8 | 0.8 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 10 | 0.8 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 10 | 0.8 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 10 | 0.8 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 1 | 0.8 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 1 | 0.8 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 1 | 0.8 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 1 | 0.8 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 1 | 0.8 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 1 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 2 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 2 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 2 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 2 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 2 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 2 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 2 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 2 | 0.8 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 2 | 0.8 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 5 | 0.8 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 5 | 0.8 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 5 | 0.8 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 5 | 0.8 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 5 | 0.8 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 5 | 0.8 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 5 | 0.8 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 5 | 0.8 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 5 | 0.8 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE1 | 6 | 0.8 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE2 | 6 | 0.8 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE1 | 6 | 0.8 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE2 | 6 | 0.8 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE1 | 6 | 0.8 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE2 | 6 | 0.8 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 2 | 0.8 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 2 | 0.8 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 2 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 2 | 0.8 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 2 | 0.8 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 2 | 0.8 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 10 | 0.79 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 10 | 0.79 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 10 | 0.79 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 10 | 0.79 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 10 | 0.79 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 10 | 0.79 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 4 | 0.79 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 4 | 0.79 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 4 | 0.79 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 9 | 0.79 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 9 | 0.79 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 9 | 0.79 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB2 | 6 | 0.79 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB3 | 6 | 0.79 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB2 | 6 | 0.79 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB3 | 6 | 0.79 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB2 | 6 | 0.79 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB3 | 6 | 0.79 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 10 | 0.79 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 10 | 0.79 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 10 | 0.79 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 10 | 0.79 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 10 | 0.79 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 10 | 0.79 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 10 | 0.79 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 10 | 0.79 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 10 | 0.79 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 4 | 0.79 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 4 | 0.79 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 4 | 0.79 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 7 | 0.78 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 7 | 0.78 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 7 | 0.78 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 8 | 0.78 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 8 | 0.78 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 8 | 0.78 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 8 | 0.78 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 8 | 0.78 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 8 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 8 | 0.78 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 2 | 0.78 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 2 | 0.78 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 2 | 0.78 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 5 | 0.78 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 5 | 0.78 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 5 | 0.78 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 9 | 0.78 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 9 | 0.78 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 9 | 0.78 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 3 | 0.78 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 3 | 0.78 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 3 | 0.78 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 3 | 0.78 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 3 | 0.78 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 3 | 0.78 |
| (2,6) | 1:16:A:ALA:HB1 | 1:17:A:GLN:H | 9 | 0.78 |
| (2,6) | 1:16:A:ALA:HB2 | 1:17:A:GLN:H | 9 | 0.78 |
| (2,6) | 1:16:A:ALA:HB3 | 1:17:A:GLN:H | 9 | 0.78 |
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE1 | 1 | 0.78 |
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE2 | 1 | 0.78 |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE1 | 1 | 0.78 |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE2 | 1 | 0.78 |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE1 | 1 | 0.78 |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE2 | 1 | 0.78 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 6 | 0.78 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 6 | 0.78 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 6 | 0.78 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 6 | 0.78 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 6 | 0.78 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 6 | 0.78 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 6 | 0.78 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 6 | 0.78 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 6 | 0.78 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 3 | 0.78 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 3 | 0.78 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 3 | 0.78 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 2 | 0.78 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 2 | 0.78 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 2 | 0.78 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 6 | 0.78 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 6 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 6 | 0.78 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 6 | 0.78 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 6 | 0.78 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 6 | 0.78 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 1 | 0.77 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 1 | 0.77 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 1 | 0.77 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 2 | 0.77 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 2 | 0.77 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 2 | 0.77 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 2 | 0.77 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 2 | 0.77 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 2 | 0.77 |
| (2,466) | 1:79:A:ILE:HG21 | 1:102:A:ILE:H | 6 | 0.77 |
| (2,466) | 1:79:A:ILE:HG22 | 1:102:A:ILE:H | 6 | 0.77 |
| (2,466) | 1:79:A:ILE:HG23 | 1:102:A:ILE:H | 6 | 0.77 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 2 | 0.77 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 2 | 0.77 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 2 | 0.77 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 3 | 0.77 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 3 | 0.77 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 3 | 0.77 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 10 | 0.77 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 10 | 0.77 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 10 | 0.77 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 6 | 0.77 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 6 | 0.77 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 6 | 0.77 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 8 | 0.77 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 8 | 0.77 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 8 | 0.77 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB1 | 6 | 0.77 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB2 | 6 | 0.77 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB3 | 6 | 0.77 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB1 | 6 | 0.77 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB2 | 6 | 0.77 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB3 | 6 | 0.77 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 6 | 0.77 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 6 | 0.77 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 6 | 0.77 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 6 | 0.77 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 6 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 6 | 0.77 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 1 | 0.77 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 1 | 0.77 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 1 | 0.77 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 1 | 0.77 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 1 | 0.77 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 1 | 0.77 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 2 | 0.76 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 2 | 0.76 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 2 | 0.76 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 2 | 0.76 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 2 | 0.76 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 2 | 0.76 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 2 | 0.76 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 2 | 0.76 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 2 | 0.76 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 2 | 0.76 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 2 | 0.76 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 2 | 0.76 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 8 | 0.76 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 8 | 0.76 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 8 | 0.76 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 8 | 0.76 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 6 | 0.76 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 6 | 0.76 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 6 | 0.76 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 2 | 0.76 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 2 | 0.76 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 2 | 0.76 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 2 | 0.76 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 6 | 0.76 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 6 | 0.76 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 6 | 0.76 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 7 | 0.76 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 7 | 0.76 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 7 | 0.76 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 4 | 0.76 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 4 | 0.76 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 4 | 0.76 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 10 | 0.76 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 10 | 0.76 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 10 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 5 | 0.76 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 5 | 0.76 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 5 | 0.76 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 7 | 0.76 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 7 | 0.76 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 7 | 0.76 |
| (2,7) | 1:16:A:ALA:HB1 | 1:18:A:ALA:H | 10 | 0.76 |
| (2,7) | 1:16:A:ALA:HB2 | 1:18:A:ALA:H | 10 | 0.76 |
| (2,7) | 1:16:A:ALA:HB3 | 1:18:A:ALA:H | 10 | 0.76 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 9 | 0.76 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 9 | 0.76 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 9 | 0.76 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 9 | 0.76 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 9 | 0.76 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 9 | 0.76 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 9 | 0.76 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 1 | 0.76 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 1 | 0.76 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 1 | 0.76 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 1 | 0.76 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 1 | 0.76 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 1 | 0.76 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 9 | 0.76 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 9 | 0.76 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 9 | 0.76 |
| (1,10) | 1:19:A:VAL:HG11 | 1:19:A:VAL:H | 3 | 0.76 |
| (1,10) | 1:19:A:VAL:HG12 | 1:19:A:VAL:H | 3 | 0.76 |
| (1,10) | 1:19:A:VAL:HG13 | 1:19:A:VAL:H | 3 | 0.76 |
| (1,10) | 1:19:A:VAL:HG21 | 1:19:A:VAL:H | 3 | 0.76 |
| (1,10) | 1:19:A:VAL:HG22 | 1:19:A:VAL:H | 3 | 0.76 |
| (1,10) | 1:19:A:VAL:HG23 | 1:19:A:VAL:H | 3 | 0.76 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD11 | 6 | 0.75 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD12 | 6 | 0.75 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD13 | 6 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 6 | 0.75 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 6 | 0.75 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 6 | 0.75 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 6 | 0.75 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 7 | 0.75 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 7 | 0.75 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 7 | 0.75 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 2 | 0.75 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 2 | 0.75 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 2 | 0.75 |
| (2,94) | 1:23:A:ILE:HD11 | 1:53:A:ASP:H | 7 | 0.75 |
| (2,94) | 1:23:A:ILE:HD12 | 1:53:A:ASP:H | 7 | 0.75 |
| (2,94) | 1:23:A:ILE:HD13 | 1:53:A:ASP:H | 7 | 0.75 |
| (2,5) | 1:16:A:ALA:HB1 | 1:17:A:GLN:HE21 | 6 | 0.75 |
| (2,5) | 1:16:A:ALA:HB2 | 1:17:A:GLN:HE21 | 6 | 0.75 |
| (2,5) | 1:16:A:ALA:HB3 | 1:17:A:GLN:HE21 | 6 | 0.75 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 2 | 0.75 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 2 | 0.75 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 2 | 0.75 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 2 | 0.75 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 2 | 0.75 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 2 | 0.75 |
| (1,1457) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 8 | 0.75 |
| (1,1457) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 8 | 0.75 |
| (1,1457) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 8 | 0.75 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 2 | 0.75 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 2 | 0.75 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 2 | 0.75 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 2 | 0.75 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 2 | 0.75 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 2 | 0.75 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 10 | 0.75 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 10 | 0.75 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 10 | 0.75 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 10 | 0.75 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 10 | 0.75 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 10 | 0.75 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 2 | 0.75 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 2 | 0.75 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 2 | 0.75 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 5 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 5 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 5 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 5 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 5 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 5 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 7 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 7 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 7 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 7 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 7 | 0.74 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 7 | 0.74 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1 | 5 | 0.74 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2 | 5 | 0.74 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1 | 5 | 0.74 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2 | 5 | 0.74 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1 | 5 | 0.74 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2 | 5 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 7 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 7 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 7 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 7 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 7 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 7 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 7 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 7 | 0.74 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 7 | 0.74 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 5 | 0.74 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 5 | 0.74 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 5 | 0.74 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 10 | 0.74 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 10 | 0.74 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 10 | 0.74 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 1 | 0.73 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 1 | 0.73 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 1 | 0.73 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 1 | 0.73 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 4 | 0.73 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 4 | 0.73 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 4 | 0.73 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 4 | 0.73 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 3 | 0.73 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 3 | 0.73 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 3 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 4 | 0.73 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 4 | 0.73 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 4 | 0.73 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 4 | 0.73 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 4 | 0.73 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 4 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 3 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 3 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 3 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 3 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 3 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 3 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 4 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 4 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 4 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 4 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 4 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 4 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 8 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 8 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 8 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 8 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 8 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 8 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 9 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 9 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 9 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 9 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 9 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 9 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 10 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 10 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 10 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 10 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 10 | 0.73 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 10 | 0.73 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 8 | 0.73 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 8 | 0.73 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 8 | 0.73 |
| (1,282) | 1:35:A:ALA:HB1 | 1:36:A:ALA:H | 10 | 0.73 |
| (1,282) | 1:35:A:ALA:HB2 | 1:36:A:ALA:H | 10 | 0.73 |
| (1,282) | 1:35:A:ALA:HB3 | 1:36:A:ALA:H | 10 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 5 | 0.73 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 5 | 0.73 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 5 | 0.73 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 9 | 0.73 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 9 | 0.73 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 9 | 0.73 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 1 | 0.72 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 1 | 0.72 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 1 | 0.72 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 1 | 0.72 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 7 | 0.72 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 7 | 0.72 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 7 | 0.72 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 7 | 0.72 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 1 | 0.72 |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 1 | 0.72 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 1 | 0.72 |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 1 | 0.72 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 1 | 0.72 |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 1 | 0.72 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 4 | 0.72 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 4 | 0.72 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 4 | 0.72 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 5 | 0.72 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 5 | 0.72 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 5 | 0.72 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 6 | 0.72 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 6 | 0.72 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 6 | 0.72 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 6 | 0.72 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 6 | 0.72 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 6 | 0.72 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 5 | 0.72 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 5 | 0.72 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 5 | 0.72 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 1 | 0.72 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 1 | 0.72 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 1 | 0.72 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 7 | 0.72 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 7 | 0.72 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 7 | 0.72 |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 8 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 8 | 0.71 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 8 | 0.71 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 8 | 0.71 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 8 | 0.71 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 8 | 0.71 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 6 | 0.71 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 6 | 0.71 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 6 | 0.71 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 7 | 0.71 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 7 | 0.71 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 7 | 0.71 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 1 | 0.71 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 1 | 0.71 |
| (1,206) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 1 | 0.71 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 4 | 0.71 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 4 | 0.71 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 4 | 0.71 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 1 | 0.71 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 1 | 0.71 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 1 | 0.71 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 2 | 0.7 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 2 | 0.7 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 2 | 0.7 |
| (2,7) | 1:16:A:ALA:HB1 | 1:18:A:ALA:H | 9 | 0.7 |
| (2,7) | 1:16:A:ALA:HB2 | 1:18:A:ALA:H | 9 | 0.7 |
| (2,7) | 1:16:A:ALA:HB3 | 1:18:A:ALA:H | 9 | 0.7 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 3 | 0.7 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 3 | 0.7 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 3 | 0.7 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 3 | 0.7 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 3 | 0.7 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 3 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 10 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 10 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 10 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 10 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 10 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 10 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 10 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 10 | 0.7 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 10 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 3 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 3 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 3 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 3 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 3 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 3 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 3 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 3 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 3 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 9 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 9 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 9 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 9 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 9 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 9 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 9 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 9 | 0.7 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 9 | 0.7 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 7 | 0.7 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 7 | 0.7 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 7 | 0.7 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 7 | 0.7 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 7 | 0.7 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 7 | 0.7 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 7 | 0.7 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 7 | 0.7 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 7 | 0.7 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 1 | 0.7 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 1 | 0.7 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 1 | 0.7 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 1 | 0.7 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 1 | 0.7 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 1 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 3 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 3 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 3 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 8 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 8 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 8 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 9 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 9 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 9 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 10 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 10 | 0.7 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 10 | 0.7 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 3 | 0.7 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 3 | 0.7 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 3 | 0.7 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 5 | 0.7 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 5 | 0.7 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 5 | 0.7 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 8 | 0.7 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 8 | 0.7 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 8 | 0.7 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 9 | 0.7 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 9 | 0.7 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 9 | 0.7 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 5 | 0.69 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 5 | 0.69 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 5 | 0.69 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 5 | 0.69 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 4 | 0.69 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 4 | 0.69 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 4 | 0.69 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD21 | 10 | 0.69 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD22 | 10 | 0.69 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD23 | 10 | 0.69 |
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD21 | 10 | 0.69 |
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD22 | 10 | 0.69 |
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD23 | 10 | 0.69 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 10 | 0.69 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 10 | 0.69 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 10 | 0.69 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 10 | 0.69 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 10 | 0.69 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 10 | 0.69 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 2 | 0.69 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 2 | 0.69 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 2 | 0.69 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 8 | 0.69 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 8 | 0.69 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 8 | 0.69 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 6 | 0.69 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 6 | 0.69 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 6 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 6 | 0.69 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 6 | 0.69 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 6 | 0.69 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 6 | 0.68 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 6 | 0.68 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 6 | 0.68 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 6 | 0.68 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB1 | 9 | 0.68 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB2 | 9 | 0.68 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB3 | 9 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 2 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 8 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 8 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 8 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 8 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 8 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 8 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 8 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 8 | 0.68 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 8 | 0.68 |
| (1,1457) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 4 | 0.68 |
| (1,1457) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 4 | 0.68 |
| (1,1457) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 4 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 1 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 1 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 1 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 1 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 1 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 1 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 2 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 2 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 2 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 2 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 2 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 2 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 3 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 3 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 3 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 3 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 3 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 3 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 7 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 7 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 7 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 7 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 7 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 7 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 8 | 0.68 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 8 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 8 | 0.68 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 8 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 8 | 0.68 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 8 | 0.68 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 1 | 0.68 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 2 | 0.68 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 2 | 0.68 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 2 | 0.68 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 2 | 0.68 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 2 | 0.68 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 2 | 0.68 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 2 | 0.68 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 2 | 0.68 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 2 | 0.68 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 6 | 0.67 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 6 | 0.67 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 6 | 0.67 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 6 | 0.67 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 10 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 10 | 0.67 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 10 | 0.67 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 10 | 0.67 |
| (2,3) | 1:13:A:THR:HG21 | 1:17:A:GLN:HE21 | 8 | 0.67 |
| (2,3) | 1:13:A:THR:HG22 | 1:17:A:GLN:HE21 | 8 | 0.67 |
| (2,3) | 1:13:A:THR:HG23 | 1:17:A:GLN:HE21 | 8 | 0.67 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD21 | 1 | 0.67 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD22 | 1 | 0.67 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD23 | 1 | 0.67 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 1 | 0.67 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 1 | 0.67 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 1 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 3 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 3 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 3 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 5 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 5 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 5 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 6 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 6 | 0.67 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 6 | 0.67 |
| (1,1091) | 1:77:A:LEU:HD11 | 1:103:A:SER:HA | 4 | 0.67 |
| (1,1091) | 1:77:A:LEU:HD12 | 1:103:A:SER:HA | 4 | 0.67 |
| (1,1091) | 1:77:A:LEU:HD13 | 1:103:A:SER:HA | 4 | 0.67 |
| (1,1091) | 1:77:A:LEU:HD21 | 1:103:A:SER:HA | 4 | 0.67 |
| (1,1091) | 1:77:A:LEU:HD22 | 1:103:A:SER:HA | 4 | 0.67 |
| (1,1091) | 1:77:A:LEU:HD23 | 1:103:A:SER:HA | 4 | 0.67 |
| (1,1068) | 1:76:A:TYR:HE1 | 1:78:A:GLN:HG2 | 10 | 0.67 |
| (1,1068) | 1:76:A:TYR:HE1 | 1:78:A:GLN:HG3 | 10 | 0.67 |
| (1,1068) | 1:76:A:TYR:HE2 | 1:78:A:GLN:HG2 | 10 | 0.67 |
| (1,1068) | 1:76:A:TYR:HE2 | 1:78:A:GLN:HG3 | 10 | 0.67 |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2 | 4 | 0.67 |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2 | 4 | 0.67 |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2 | 4 | 0.67 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 1 | 0.67 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 1 | 0.67 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 1 | 0.67 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 1 | 0.67 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 1 | 0.67 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 1 | 0.67 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 9 | 0.66 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 9 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 9 | 0.66 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD21 | 7 | 0.66 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD22 | 7 | 0.66 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD23 | 7 | 0.66 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD11 | 6 | 0.66 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD12 | 6 | 0.66 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD13 | 6 | 0.66 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 10 | 0.66 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 10 | 0.66 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 10 | 0.66 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 10 | 0.66 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 10 | 0.66 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 10 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 3 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 4 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 7 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 9 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 9 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 9 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 9 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 9 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 9 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 9 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 9 | 0.66 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 9 | 0.66 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 7 | 0.66 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 7 | 0.66 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 7 | 0.66 |
| (1,2016) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HD1 | 5 | 0.66 |
| (1,2016) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HD2 | 5 | 0.66 |
| (1,2016) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HD1 | 5 | 0.66 |
| (1,2016) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HD2 | 5 | 0.66 |
| (1,2016) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HD1 | 5 | 0.66 |
| (1,2016) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HD2 | 5 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 7 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 9 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 9 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 9 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 9 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 9 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 9 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 9 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 9 | 0.66 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 9 | 0.66 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 8 | 0.66 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 8 | 0.66 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 8 | 0.66 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 9 | 0.66 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 9 | 0.66 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 9 | 0.66 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 6 | 0.66 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 6 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 6 | 0.66 |
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE1 | 5 | 0.65 |
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE2 | 5 | 0.65 |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE1 | 5 | 0.65 |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE2 | 5 | 0.65 |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE1 | 5 | 0.65 |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE2 | 5 | 0.65 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 8 | 0.65 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 8 | 0.65 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 8 | 0.65 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 8 | 0.65 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 9 | 0.65 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 9 | 0.65 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 9 | 0.65 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 9 | 0.65 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 3 | 0.65 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 3 | 0.65 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 3 | 0.65 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD21 | 9 | 0.65 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD22 | 9 | 0.65 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD23 | 9 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 3 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 3 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 3 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 3 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 3 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 3 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 5 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 5 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 5 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 5 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 5 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 5 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 9 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 9 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 9 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 9 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 9 | 0.65 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 9 | 0.65 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 5 | 0.65 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 5 | 0.65 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 5 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 5 | 0.65 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 5 | 0.65 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 5 | 0.65 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 5 | 0.65 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 5 | 0.65 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 5 | 0.65 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 8 | 0.65 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 8 | 0.65 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 8 | 0.65 |
| (1,1788) | 1:125:A:LYS:HB2 | 1:125:A:LYS:HE2 | 7 | 0.65 |
| (1,1788) | 1:125:A:LYS:HB2 | 1:125:A:LYS:HE3 | 7 | 0.65 |
| (1,1788) | 1:125:A:LYS:HB3 | 1:125:A:LYS:HE2 | 7 | 0.65 |
| (1,1788) | 1:125:A:LYS:HB3 | 1:125:A:LYS:HE3 | 7 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 8 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 8 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 8 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 8 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 8 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 8 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 8 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 8 | 0.65 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 8 | 0.65 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 7 | 0.65 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 7 | 0.65 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 7 | 0.65 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 10 | 0.65 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 10 | 0.65 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 10 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 6 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 6 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 6 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 6 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 6 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 6 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 6 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 6 | 0.65 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 6 | 0.65 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 5 | 0.65 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 5 | 0.65 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 5 | 0.65 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 5 | 0.65 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 5 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 5 | 0.65 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 6 | 0.65 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 6 | 0.65 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 6 | 0.65 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 6 | 0.65 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 6 | 0.65 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 6 | 0.65 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 4 | 0.65 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 8 | 0.65 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 8 | 0.65 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 8 | 0.65 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 8 | 0.65 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 8 | 0.65 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 8 | 0.65 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 8 | 0.65 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 8 | 0.65 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 8 | 0.65 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 8 | 0.64 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 8 | 0.64 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 8 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 6 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 6 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 6 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 6 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 6 | 0.64 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 6 | 0.64 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1 | 10 | 0.64 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2 | 10 | 0.64 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1 | 10 | 0.64 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2 | 10 | 0.64 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1 | 10 | 0.64 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2 | 10 | 0.64 |
| (1,923) | 1:70:A:LEU:HD11 | 1:71:A:LYS:H | 2 | 0.64 |
| (1,923) | 1:70:A:LEU:HD12 | 1:71:A:LYS:H | 2 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,923) | 1:70:A:LEU:HD13 | 1:71:A:LYS:H | 2 | 0.64 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 5 | 0.64 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 5 | 0.64 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 5 | 0.64 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD11 | 2 | 0.64 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD12 | 2 | 0.64 |
| (1,145) | 1:28:A:HIS:HE1 | 1:48:A:ILE:HD13 | 2 | 0.64 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 5 | 0.63 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 5 | 0.63 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 5 | 0.63 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 5 | 0.63 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 5 | 0.63 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 10 | 0.63 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 10 | 0.63 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 10 | 0.63 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 10 | 0.63 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 10 | 0.63 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 10 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 1 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 1 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 1 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 1 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 1 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 1 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 1 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 1 | 0.63 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 1 | 0.63 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 9 | 0.63 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 9 | 0.63 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 9 | 0.63 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 9 | 0.63 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 9 | 0.63 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 9 | 0.63 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD11 | 5 | 0.63 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD12 | 5 | 0.63 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD13 | 5 | 0.63 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 2 | 0.63 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 2 | 0.63 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 2 | 0.63 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 9 | 0.63 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 9 | 0.63 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 9 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 1 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 1 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 1 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 1 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 1 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 1 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 1 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 1 | 0.63 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 1 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 10 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 10 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 10 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 10 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 10 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 10 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 10 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 10 | 0.63 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 10 | 0.63 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD11 | 3 | 0.63 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD12 | 3 | 0.63 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD13 | 3 | 0.63 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD11 | 3 | 0.63 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD12 | 3 | 0.63 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD13 | 3 | 0.63 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG11 | 8 | 0.63 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG12 | 8 | 0.63 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG13 | 8 | 0.63 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 4 | 0.63 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 4 | 0.63 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 4 | 0.63 |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H | 4 | 0.62 |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H | 4 | 0.62 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 9 | 0.62 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 9 | 0.62 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 9 | 0.62 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB1 | 3 | 0.62 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB2 | 3 | 0.62 |
| (2,184) | 1:37:A:GLY:H | 1:38:A:ALA:HB3 | 3 | 0.62 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 5 | 0.62 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 5 | 0.62 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 5 | 0.62 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 5 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 5 | 0.62 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 5 | 0.62 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD21 | 6 | 0.62 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD22 | 6 | 0.62 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD23 | 6 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 3 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 3 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 3 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 4 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 4 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 4 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 5 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 5 | 0.62 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 5 | 0.62 |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ | 2 | 0.62 |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ | 2 | 0.62 |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ | 2 | 0.62 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD11 | 5 | 0.62 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD12 | 5 | 0.62 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD13 | 5 | 0.62 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD11 | 5 | 0.62 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD12 | 5 | 0.62 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD13 | 5 | 0.62 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG11 | 10 | 0.62 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG12 | 10 | 0.62 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG13 | 10 | 0.62 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE1 | 2 | 0.62 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE2 | 2 | 0.62 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE1 | 2 | 0.62 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE2 | 2 | 0.62 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE1 | 2 | 0.62 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE2 | 2 | 0.62 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 9 | 0.61 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 9 | 0.61 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 9 | 0.61 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 9 | 0.61 |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 5 | 0.61 |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 5 | 0.61 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 5 | 0.61 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 2 | 0.61 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 2 | 0.61 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 2 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 2 | 0.61 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 3 | 0.61 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 3 | 0.61 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 3 | 0.61 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 7 | 0.61 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 7 | 0.61 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 7 | 0.61 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 7 | 0.61 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 7 | 0.61 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 7 | 0.61 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD11 | 4 | 0.61 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD12 | 4 | 0.61 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD13 | 4 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 5 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 5 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 5 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 5 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 5 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 5 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 5 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 5 | 0.61 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 5 | 0.61 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG21 | 3 | 0.61 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG22 | 3 | 0.61 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG23 | 3 | 0.61 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG21 | 3 | 0.61 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG22 | 3 | 0.61 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG23 | 3 | 0.61 |
| (1,1274) | 1:82:A:THR:HG21 | 1:96:A:SER:HB3 | 10 | 0.61 |
| (1,1274) | 1:82:A:THR:HG22 | 1:96:A:SER:HB3 | 10 | 0.61 |
| (1,1274) | 1:82:A:THR:HG23 | 1:96:A:SER:HB3 | 10 | 0.61 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 4 | 0.61 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 4 | 0.61 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 4 | 0.61 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 4 | 0.61 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 4 | 0.61 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 4 | 0.61 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 1 | 0.61 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 1 | 0.61 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 7 | 0.61 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 7 | 0.61 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 7 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 7 | 0.6 |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 1 | 0.6 |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 1 | 0.6 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 1 | 0.6 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 3 | 0.6 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 3 | 0.6 |
| (2,94) | 1:23:A:ILE:HD11 | 1:53:A:ASP:H | 8 | 0.6 |
| (2,94) | 1:23:A:ILE:HD12 | 1:53:A:ASP:H | 8 | 0.6 |
| (2,94) | 1:23:A:ILE:HD13 | 1:53:A:ASP:H | 8 | 0.6 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 6 | 0.6 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 6 | 0.6 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 6 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 10 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 10 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 10 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 10 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 10 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 10 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 10 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 10 | 0.6 |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 10 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 1 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 1 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 1 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 4 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 4 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 4 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 5 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 5 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 5 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 7 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 7 | 0.6 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 7 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 1 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 1 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 1 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 2 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 2 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 2 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 4 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 4 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 4 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 10 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 10 | 0.6 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 10 | 0.6 |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H | 8 | 0.6 |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H | 8 | 0.6 |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H | 8 | 0.6 |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H | 8 | 0.6 |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H | 8 | 0.6 |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H | 8 | 0.6 |
| (1,923) | 1:70:A:LEU:HD11 | 1:71:A:LYS:H | 1 | 0.6 |
| (1,923) | 1:70:A:LEU:HD12 | 1:71:A:LYS:H | 1 | 0.6 |
| (1,923) | 1:70:A:LEU:HD13 | 1:71:A:LYS:H | 1 | 0.6 |
| (1,650) | 1:58:A:VAL:HG11 | 1:58:A:VAL:H | 3 | 0.6 |
| (1,650) | 1:58:A:VAL:HG12 | 1:58:A:VAL:H | 3 | 0.6 |
| (1,650) | 1:58:A:VAL:HG13 | 1:58:A:VAL:H | 3 | 0.6 |
| (1,650) | 1:58:A:VAL:HG21 | 1:58:A:VAL:H | 3 | 0.6 |
| (1,650) | 1:58:A:VAL:HG22 | 1:58:A:VAL:H | 3 | 0.6 |
| (1,650) | 1:58:A:VAL:HG23 | 1:58:A:VAL:H | 3 | 0.6 |
| (1,650) | 1:58:A:VAL:HG11 | 1:58:A:VAL:H | 5 | 0.6 |
| (1,650) | 1:58:A:VAL:HG12 | 1:58:A:VAL:H | 5 | 0.6 |
| (1,650) | 1:58:A:VAL:HG13 | 1:58:A:VAL:H | 5 | 0.6 |
| (1,650) | 1:58:A:VAL:HG21 | 1:58:A:VAL:H | 5 | 0.6 |
| (1,650) | 1:58:A:VAL:HG22 | 1:58:A:VAL:H | 5 | 0.6 |
| (1,650) | 1:58:A:VAL:HG23 | 1:58:A:VAL:H | 5 | 0.6 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 1 | 0.59 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 1 | 0.59 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 8 | 0.59 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 8 | 0.59 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 2 | 0.59 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 2 | 0.59 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 2 | 0.59 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 2 | 0.59 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 2 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2355) | 1:173:A:VAL:HG21 | 1:173:A:VAL:H | 6 | 0.59 |
| (1,2355) | 1:173:A:VAL:HG22 | 1:173:A:VAL:H | 6 | 0.59 |
| (1,2355) | 1:173:A:VAL:HG23 | 1:173:A:VAL:H | 6 | 0.59 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 1 | 0.59 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 1 | 0.59 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 1 | 0.59 |
| (1,2287) | 1:168:A:PHE:HD1 | 1:169:A:ASP:H | 2 | 0.59 |
| (1,2287) | 1:168:A:PHE:HD2 | 1:169:A:ASP:H | 2 | 0.59 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 2 | 0.59 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 2 | 0.59 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 2 | 0.59 |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H | 3 | 0.59 |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H | 3 | 0.59 |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H | 3 | 0.59 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 2 | 0.59 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 2 | 0.59 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 2 | 0.59 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 3 | 0.59 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 3 | 0.59 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 3 | 0.59 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG21 | 10 | 0.59 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG22 | 10 | 0.59 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG23 | 10 | 0.59 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG21 | 10 | 0.59 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG22 | 10 | 0.59 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG23 | 10 | 0.59 |
| (1,1275) | 1:82:A:THR:HG21 | 1:96:A:SER:HB2 | 1 | 0.59 |
| (1,1275) | 1:82:A:THR:HG22 | 1:96:A:SER:HB2 | 1 | 0.59 |
| (1,1275) | 1:82:A:THR:HG23 | 1:96:A:SER:HB2 | 1 | 0.59 |
| (1,1275) | 1:82:A:THR:HG21 | 1:96:A:SER:HB2 | 4 | 0.59 |
| (1,1275) | 1:82:A:THR:HG22 | 1:96:A:SER:HB2 | 4 | 0.59 |
| (1,1275) | 1:82:A:THR:HG23 | 1:96:A:SER:HB2 | 4 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 1 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 1 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 1 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 1 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 1 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 1 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 1 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 1 | 0.59 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 1 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 7 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 7 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 7 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 8 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 8 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 8 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 9 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 9 | 0.59 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 9 | 0.59 |
| (1,923) | 1:70:A:LEU:HD11 | 1:71:A:LYS:H | 7 | 0.59 |
| (1,923) | 1:70:A:LEU:HD12 | 1:71:A:LYS:H | 7 | 0.59 |
| (1,923) | 1:70:A:LEU:HD13 | 1:71:A:LYS:H | 7 | 0.59 |
| (1,508) | 1:48:A:ILE:HG21 | 1:153:A:ILE:HG13 | 8 | 0.59 |
| (1,508) | 1:48:A:ILE:HG22 | 1:153:A:ILE:HG13 | 8 | 0.59 |
| (1,508) | 1:48:A:ILE:HG23 | 1:153:A:ILE:HG13 | 8 | 0.59 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 3 | 0.59 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 3 | 0.59 |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 3 | 0.59 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 3 | 0.59 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 3 | 0.59 |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 3 | 0.59 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 3 | 0.59 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 3 | 0.59 |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 3 | 0.59 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 8 | 0.59 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 8 | 0.59 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 8 | 0.59 |
| (1,282) | 1:35:A:ALA:HB1 | 1:36:A:ALA:H | 1 | 0.59 |
| (1,282) | 1:35:A:ALA:HB2 | 1:36:A:ALA:H | 1 | 0.59 |
| (1,282) | 1:35:A:ALA:HB3 | 1:36:A:ALA:H | 1 | 0.59 |
| (2,766) | 1:169:A:ASP:H | 1:171:A:LEU:HD21 | 2 | 0.58 |
| (2,766) | 1:169:A:ASP:H | 1:171:A:LEU:HD22 | 2 | 0.58 |
| (2,766) | 1:169:A:ASP:H | 1:171:A:LEU:HD23 | 2 | 0.58 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 9 | 0.58 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 9 | 0.58 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 10 | 0.58 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 10 | 0.58 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 10 | 0.58 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD11 | 6 | 0.58 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD12 | 6 | 0.58 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD13 | 6 | 0.58 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD11 | 8 | 0.58 |
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD12 | 8 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1884) | 1:134:A:TRP:HA | 1:143:A:ILE:HD13 | 8 | 0.58 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 10 | 0.58 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 10 | 0.58 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 10 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 2 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 2 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 2 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 2 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 2 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 2 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 2 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 2 | 0.58 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 2 | 0.58 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD11 | 3 | 0.58 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD12 | 3 | 0.58 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD13 | 3 | 0.58 |
| (1,1274) | 1:82:A:THR:HG21 | 1:96:A:SER:HB3 | 5 | 0.58 |
| (1,1274) | 1:82:A:THR:HG22 | 1:96:A:SER:HB3 | 5 | 0.58 |
| (1,1274) | 1:82:A:THR:HG23 | 1:96:A:SER:HB3 | 5 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 3 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 3 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 3 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 5 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 5 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 5 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG21 | 6 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG22 | 6 | 0.58 |
| (1,1206) | 1:81:A:ILE:HA | 1:81:A:ILE:HG23 | 6 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3 | 1 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3 | 1 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3 | 1 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3 | 1 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3 | 1 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3 | 1 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3 | 2 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3 | 2 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3 | 2 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3 | 2 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3 | 2 | 0.58 |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3 | 2 | 0.58 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2 | 9 | 0.58 |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3 | 9 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2 | 9 | 0.58 |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3 | 9 | 0.58 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2 | 9 | 0.58 |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3 | 9 | 0.58 |
| (1,508) | 1:48:A:ILE:HG21 | 1:153:A:ILE:HG13 | 3 | 0.58 |
| (1,508) | 1:48:A:ILE:HG22 | 1:153:A:ILE:HG13 | 3 | 0.58 |
| (1,508) | 1:48:A:ILE:HG23 | 1:153:A:ILE:HG13 | 3 | 0.58 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 5 | 0.57 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 5 | 0.57 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 5 | 0.57 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 6 | 0.57 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 6 | 0.57 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 6 | 0.57 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 4 | 0.57 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 4 | 0.57 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 6 | 0.57 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 6 | 0.57 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD21 | 7 | 0.57 |
| (2,520) | 1:84:A:GLY:HA2 | 1:155:A:ASN:HD22 | 7 | 0.57 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD21 | 7 | 0.57 |
| (2,520) | 1:84:A:GLY:HA3 | 1:155:A:ASN:HD22 | 7 | 0.57 |
| (2,507) | 1:82:A:THR:H | 1:156:A:PHE:HD1 | 1 | 0.57 |
| (2,507) | 1:82:A:THR:H | 1:156:A:PHE:HD2 | 1 | 0.57 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 1 | 0.57 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 1 | 0.57 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 6 | 0.57 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 6 | 0.57 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 10 | 0.57 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 10 | 0.57 |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA | 4 | 0.57 |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA | 4 | 0.57 |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA | 4 | 0.57 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 3 | 0.57 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 3 | 0.57 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 6 | 0.57 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 6 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 1 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 1 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 4 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 4 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 6 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 6 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 8 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 8 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 10 | 0.57 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 10 | 0.57 |
| (2,7) | 1:16:A:ALA:HB1 | 1:18:A:ALA:H | 7 | 0.57 |
| (2,7) | 1:16:A:ALA:HB2 | 1:18:A:ALA:H | 7 | 0.57 |
| (2,7) | 1:16:A:ALA:HB3 | 1:18:A:ALA:H | 7 | 0.57 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 3 | 0.57 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 3 | 0.57 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 3 | 0.57 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 7 | 0.57 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 7 | 0.57 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 7 | 0.57 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD11 | 8 | 0.57 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD12 | 8 | 0.57 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD13 | 8 | 0.57 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD11 | 8 | 0.57 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD12 | 8 | 0.57 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD13 | 8 | 0.57 |
| (1,508) | 1:48:A:ILE:HG21 | 1:153:A:ILE:HG13 | 2 | 0.57 |
| (1,508) | 1:48:A:ILE:HG22 | 1:153:A:ILE:HG13 | 2 | 0.57 |
| (1,508) | 1:48:A:ILE:HG23 | 1:153:A:ILE:HG13 | 2 | 0.57 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 9 | 0.57 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 9 | 0.57 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 9 | 0.57 |
| (1,282) | 1:35:A:ALA:HB1 | 1:36:A:ALA:H | 6 | 0.57 |
| (1,282) | 1:35:A:ALA:HB2 | 1:36:A:ALA:H | 6 | 0.57 |
| (1,282) | 1:35:A:ALA:HB3 | 1:36:A:ALA:H | 6 | 0.57 |
| (1,166) | 1:29:A:LEU:HD11 | 1:175:A:PHE:H | 1 | 0.57 |
| (1,166) | 1:29:A:LEU:HD12 | 1:175:A:PHE:H | 1 | 0.57 |
| (1,166) | 1:29:A:LEU:HD13 | 1:175:A:PHE:H | 1 | 0.57 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 4 | 0.56 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 4 | 0.56 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 4 | 0.56 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 7 | 0.56 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 7 | 0.56 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 7 | 0.56 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 3 | 0.56 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 3 | 0.56 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 3 | 0.56 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 3 | 0.56 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 7 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 7 | 0.56 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 7 | 0.56 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 7 | 0.56 |
| (2,721) | 1:144:A:VAL:HA | 1:145:A:TYR:HD1 | 6 | 0.56 |
| (2,721) | 1:144:A:VAL:HA | 1:145:A:TYR:HD2 | 6 | 0.56 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 2 | 0.56 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 2 | 0.56 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 9 | 0.56 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 9 | 0.56 |
| (2,618) | 1:119:A:ALA:HB1 | 1:149:A:LYS:H | 6 | 0.56 |
| (2,618) | 1:119:A:ALA:HB2 | 1:149:A:LYS:H | 6 | 0.56 |
| (2,618) | 1:119:A:ALA:HB3 | 1:149:A:LYS:H | 6 | 0.56 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 4 | 0.56 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 4 | 0.56 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 6 | 0.56 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 6 | 0.56 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 10 | 0.56 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 10 | 0.56 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 7 | 0.56 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 7 | 0.56 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 7 | 0.56 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 7 | 0.56 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 3 | 0.56 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 3 | 0.56 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 8 | 0.56 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 8 | 0.56 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 8 | 0.56 |
| (2,7) | 1:16:A:ALA:HB1 | 1:18:A:ALA:H | 4 | 0.56 |
| (2,7) | 1:16:A:ALA:HB2 | 1:18:A:ALA:H | 4 | 0.56 |
| (2,7) | 1:16:A:ALA:HB3 | 1:18:A:ALA:H | 4 | 0.56 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 4 | 0.56 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 4 | 0.56 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 4 | 0.56 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 4 | 0.56 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 4 | 0.56 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 4 | 0.56 |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H | 9 | 0.56 |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H | 9 | 0.56 |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H | 9 | 0.56 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 3 | 0.56 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 3 | 0.56 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 3 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 3 | 0.56 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 3 | 0.56 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 3 | 0.56 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 3 | 0.56 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 3 | 0.56 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 3 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 4 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 4 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 4 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 4 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 4 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 4 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 4 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 4 | 0.56 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 4 | 0.56 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD11 | 10 | 0.56 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD12 | 10 | 0.56 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD13 | 10 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HD1 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HD2 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HD1 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HD2 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HD1 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HD2 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HD1 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HD2 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HD1 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HD2 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HD1 | 2 | 0.56 |
| (1,1099) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HD2 | 2 | 0.56 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 2 | 0.56 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 2 | 0.56 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 2 | 0.56 |
| (1,282) | 1:35:A:ALA:HB1 | 1:36:A:ALA:H | 5 | 0.56 |
| (1,282) | 1:35:A:ALA:HB2 | 1:36:A:ALA:H | 5 | 0.56 |
| (1,282) | 1:35:A:ALA:HB3 | 1:36:A:ALA:H | 5 | 0.56 |
| (1,282) | 1:35:A:ALA:HB1 | 1:36:A:ALA:H | 7 | 0.56 |
| (1,282) | 1:35:A:ALA:HB2 | 1:36:A:ALA:H | 7 | 0.56 |
| (1,282) | 1:35:A:ALA:HB3 | 1:36:A:ALA:H | 7 | 0.56 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 5 | 0.56 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 5 | 0.56 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 10 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 10 | 0.56 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 10 | 0.56 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 8 | 0.55 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 8 | 0.55 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 8 | 0.55 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 6 | 0.55 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 6 | 0.55 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 7 | 0.55 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 7 | 0.55 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 5 | 0.55 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 5 | 0.55 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 5 | 0.55 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 5 | 0.55 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 9 | 0.55 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 9 | 0.55 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 1 | 0.55 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 1 | 0.55 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 1 | 0.55 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 2 | 0.55 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 2 | 0.55 |
| (2,367) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HG11 | 6 | 0.55 |
| (2,367) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HG12 | 6 | 0.55 |
| (2,367) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HG13 | 6 | 0.55 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 5 | 0.55 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 5 | 0.55 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 5 | 0.55 |
| (2,5) | 1:16:A:ALA:HB1 | 1:17:A:GLN:HE21 | 3 | 0.55 |
| (2,5) | 1:16:A:ALA:HB2 | 1:17:A:GLN:HE21 | 3 | 0.55 |
| (2,5) | 1:16:A:ALA:HB3 | 1:17:A:GLN:HE21 | 3 | 0.55 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 4 | 0.55 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 4 | 0.55 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 4 | 0.55 |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H | 4 | 0.55 |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H | 4 | 0.55 |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H | 4 | 0.55 |
| (1,1274) | 1:82:A:THR:HG21 | 1:96:A:SER:HB3 | 2 | 0.55 |
| (1,1274) | 1:82:A:THR:HG22 | 1:96:A:SER:HB3 | 2 | 0.55 |
| (1,1274) | 1:82:A:THR:HG23 | 1:96:A:SER:HB3 | 2 | 0.55 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD11 | 4 | 0.55 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD12 | 4 | 0.55 |
| (1,991) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD13 | 4 | 0.55 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD11 | 4 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD12 | 4 | 0.55 |
| (1,991) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD13 | 4 | 0.55 |
| (1,923) | 1:70:A:LEU:HD11 | 1:71:A:LYS:H | 6 | 0.55 |
| (1,923) | 1:70:A:LEU:HD12 | 1:71:A:LYS:H | 6 | 0.55 |
| (1,923) | 1:70:A:LEU:HD13 | 1:71:A:LYS:H | 6 | 0.55 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG11 | 9 | 0.55 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG12 | 9 | 0.55 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG13 | 9 | 0.55 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 2 | 0.55 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 2 | 0.55 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 3 | 0.55 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 3 | 0.55 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 6 | 0.55 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 6 | 0.55 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 3 | 0.54 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 3 | 0.54 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 4 | 0.54 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 4 | 0.54 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 5 | 0.54 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 5 | 0.54 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 3 | 0.54 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 3 | 0.54 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 3 | 0.54 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 3 | 0.54 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 6 | 0.54 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 6 | 0.54 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 6 | 0.54 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 7 | 0.54 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 7 | 0.54 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 8 | 0.54 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 8 | 0.54 |
| (2,397) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HA | 6 | 0.54 |
| (2,397) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HA | 6 | 0.54 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 2 | 0.54 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 2 | 0.54 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 10 | 0.54 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 10 | 0.54 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 5 | 0.54 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 5 | 0.54 |
| (1,2069) | 1:148:A:THR:HG21 | 1:148:A:THR:H | 7 | 0.54 |
| (1,2069) | 1:148:A:THR:HG22 | 1:148:A:THR:H | 7 | 0.54 |
| (1,2069) | 1:148:A:THR:HG23 | 1:148:A:THR:H | 7 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H | 8 | 0.54 |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H | 8 | 0.54 |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H | 8 | 0.54 |
| (1,2009) | 1:142:A:ILE:HD11 | 1:142:A:ILE:H | 6 | 0.54 |
| (1,2009) | 1:142:A:ILE:HD12 | 1:142:A:ILE:H | 6 | 0.54 |
| (1,2009) | 1:142:A:ILE:HD13 | 1:142:A:ILE:H | 6 | 0.54 |
| (1,1895) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HD11 | 1 | 0.54 |
| (1,1895) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HD12 | 1 | 0.54 |
| (1,1895) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HD13 | 1 | 0.54 |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H | 10 | 0.54 |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H | 10 | 0.54 |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H | 10 | 0.54 |
| (1,1544) | 1:102:A:ILE:HG21 | 1:103:A:SER:H | 4 | 0.54 |
| (1,1544) | 1:102:A:ILE:HG22 | 1:103:A:SER:H | 4 | 0.54 |
| (1,1544) | 1:102:A:ILE:HG23 | 1:103:A:SER:H | 4 | 0.54 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD21 | 8 | 0.54 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD22 | 8 | 0.54 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD23 | 8 | 0.54 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD11 | 5 | 0.54 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD12 | 5 | 0.54 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD13 | 5 | 0.54 |
| (1,700) | 1:61:A:LYS:HE2 | 1:108:A:SER:HB2 | 10 | 0.54 |
| (1,700) | 1:61:A:LYS:HE2 | 1:108:A:SER:HB3 | 10 | 0.54 |
| (1,700) | 1:61:A:LYS:HE3 | 1:108:A:SER:HB2 | 10 | 0.54 |
| (1,700) | 1:61:A:LYS:HE3 | 1:108:A:SER:HB3 | 10 | 0.54 |
| (1,650) | 1:58:A:VAL:HG11 | 1:58:A:VAL:H | 6 | 0.54 |
| (1,650) | 1:58:A:VAL:HG12 | 1:58:A:VAL:H | 6 | 0.54 |
| (1,650) | 1:58:A:VAL:HG13 | 1:58:A:VAL:H | 6 | 0.54 |
| (1,650) | 1:58:A:VAL:HG21 | 1:58:A:VAL:H | 6 | 0.54 |
| (1,650) | 1:58:A:VAL:HG22 | 1:58:A:VAL:H | 6 | 0.54 |
| (1,650) | 1:58:A:VAL:HG23 | 1:58:A:VAL:H | 6 | 0.54 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 3 | 0.54 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 3 | 0.54 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 3 | 0.54 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 1 | 0.53 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 1 | 0.53 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 1 | 0.53 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 8 | 0.53 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 8 | 0.53 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE1 | 6 | 0.53 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE2 | 6 | 0.53 |
| (2,661) | 1:125:A:LYS:HG2 | 1:126:A:THR:H | 3 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,661) | 1:125:A:LYS:HG3 | 1:126:A:THR:H | 3 | 0.53 |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H | 1 | 0.53 |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H | 1 | 0.53 |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H | 3 | 0.53 |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H | 3 | 0.53 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 7 | 0.53 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 7 | 0.53 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 8 | 0.53 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 8 | 0.53 |
| (2,534) | 1:85:A:TYR:HE1 | 1:151:A:VAL:H | 5 | 0.53 |
| (2,534) | 1:85:A:TYR:HE2 | 1:151:A:VAL:H | 5 | 0.53 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 4 | 0.53 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 4 | 0.53 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 4 | 0.53 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 4 | 0.53 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 4 | 0.53 |
| (2,473) | 1:80:A:GLN:HB2 | 1:101:A:VAL:HA | 5 | 0.53 |
| (2,473) | 1:80:A:GLN:HB3 | 1:101:A:VAL:HA | 5 | 0.53 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 9 | 0.53 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 9 | 0.53 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 2 | 0.53 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 2 | 0.53 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 3 | 0.53 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 3 | 0.53 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 8 | 0.53 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 8 | 0.53 |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H | 4 | 0.53 |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H | 4 | 0.53 |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H | 4 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 3 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 3 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 3 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 6 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 6 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 6 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 7 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 7 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 7 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 9 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 9 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 9 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 10 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 10 | 0.53 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 10 | 0.53 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD21 | 4 | 0.53 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD22 | 4 | 0.53 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD23 | 4 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD11 | 1 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD12 | 1 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD13 | 1 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD11 | 3 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD12 | 3 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD13 | 3 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD11 | 6 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD12 | 6 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD13 | 6 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD11 | 9 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD12 | 9 | 0.53 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD13 | 9 | 0.53 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG11 | 5 | 0.53 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG12 | 5 | 0.53 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG13 | 5 | 0.53 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 2 | 0.53 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 2 | 0.53 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 2 | 0.53 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 8 | 0.53 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 8 | 0.53 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 8 | 0.53 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 1 | 0.53 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 1 | 0.53 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 1 | 0.53 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 2 | 0.53 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 2 | 0.53 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 2 | 0.53 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 5 | 0.53 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 5 | 0.53 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 5 | 0.53 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 6 | 0.53 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 6 | 0.53 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 6 | 0.53 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 8 | 0.53 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 8 | 0.53 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 8 | 0.53 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 9 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 9 | 0.53 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 9 | 0.53 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 2 | 0.52 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 2 | 0.52 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 2 | 0.52 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 3 | 0.52 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 3 | 0.52 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 3 | 0.52 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 3 | 0.52 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 3 | 0.52 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD11 | 1 | 0.52 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD12 | 1 | 0.52 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD13 | 1 | 0.52 |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H | 6 | 0.52 |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H | 6 | 0.52 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 4 | 0.52 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 4 | 0.52 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 4 | 0.52 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 4 | 0.52 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 9 | 0.52 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 9 | 0.52 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 9 | 0.52 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 9 | 0.52 |
| (2,443) | 1:76:A:TYR:HE1 | 1:78:A:GLN:HE22 | 10 | 0.52 |
| (2,443) | 1:76:A:TYR:HE2 | 1:78:A:GLN:HE22 | 10 | 0.52 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD1 | 9 | 0.52 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD2 | 9 | 0.52 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 1 | 0.52 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 1 | 0.52 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 7 | 0.52 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 7 | 0.52 |
| (2,350) | 1:63:A:THR:HA | 1:175:A:PHE:HE1 | 6 | 0.52 |
| (2,350) | 1:63:A:THR:HA | 1:175:A:PHE:HE2 | 6 | 0.52 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 9 | 0.52 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 9 | 0.52 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 4 | 0.52 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 4 | 0.52 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 5 | 0.52 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 5 | 0.52 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 9 | 0.52 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 9 | 0.52 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 10 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 10 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 1 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 1 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 1 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 6 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 6 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 6 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 8 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 8 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 8 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 9 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 9 | 0.52 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 9 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 3 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 3 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 3 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 3 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 3 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 3 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 3 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 3 | 0.52 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 3 | 0.52 |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H | 10 | 0.52 |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H | 10 | 0.52 |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H | 10 | 0.52 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 2 | 0.52 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 2 | 0.52 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 2 | 0.52 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 9 | 0.52 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 9 | 0.52 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 9 | 0.52 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 1 | 0.52 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 1 | 0.52 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 1 | 0.52 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 3 | 0.52 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 3 | 0.52 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 3 | 0.52 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 9 | 0.52 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 9 | 0.52 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 9 | 0.52 |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA | 5 | 0.52 |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA | 5 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA | 5 | 0.52 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD11 | 2 | 0.52 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD12 | 2 | 0.52 |
| (1,1103) | 1:77:A:LEU:H | 1:104:A:LEU:HD13 | 2 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H | 3 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H | 3 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H | 3 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H | 3 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H | 3 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H | 3 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H | 4 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H | 4 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H | 4 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H | 4 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H | 4 | 0.52 |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H | 4 | 0.52 |
| (1,288) | 1:36:A:ALA:HB1 | 1:37:A:GLY:H | 1 | 0.52 |
| (1,288) | 1:36:A:ALA:HB2 | 1:37:A:GLY:H | 1 | 0.52 |
| (1,288) | 1:36:A:ALA:HB3 | 1:37:A:GLY:H | 1 | 0.52 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 10 | 0.52 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 10 | 0.52 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 10 | 0.51 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 10 | 0.51 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 10 | 0.51 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 5 | 0.51 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 5 | 0.51 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 9 | 0.51 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 9 | 0.51 |
| (2,716) | 1:142:A:ILE:HB | 1:145:A:TYR:HE1 | 5 | 0.51 |
| (2,716) | 1:142:A:ILE:HB | 1:145:A:TYR:HE2 | 5 | 0.51 |
| (2,716) | 1:142:A:ILE:HB | 1:145:A:TYR:HE1 | 6 | 0.51 |
| (2,716) | 1:142:A:ILE:HB | 1:145:A:TYR:HE2 | 6 | 0.51 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE1 | 9 | 0.51 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE2 | 9 | 0.51 |
| (2,700) | 1:132:A:SER:HB3 | 1:145:A:TYR:HE1 | 1 | 0.51 |
| (2,700) | 1:132:A:SER:HB3 | 1:145:A:TYR:HE2 | 1 | 0.51 |
| (2,700) | 1:132:A:SER:HB3 | 1:145:A:TYR:HE1 | 2 | 0.51 |
| (2,700) | 1:132:A:SER:HB3 | 1:145:A:TYR:HE2 | 2 | 0.51 |
| (2,631) | 1:122:A:TYR:HD1 | 1:124:A:ASP:H | 7 | 0.51 |
| (2,631) | 1:122:A:TYR:HD2 | 1:124:A:ASP:H | 7 | 0.51 |
| (2,631) | 1:122:A:TYR:HD1 | 1:124:A:ASP:H | 8 | 0.51 |
| (2,631) | 1:122:A:TYR:HD2 | 1:124:A:ASP:H | 8 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 4 | 0.51 |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 4 | 0.51 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 4 | 0.51 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG2 | 9 | 0.51 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG3 | 9 | 0.51 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 1 | 0.51 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 1 | 0.51 |
| (2,535) | 1:85:A:TYR:HE1 | 1:153:A:ILE:H | 3 | 0.51 |
| (2,535) | 1:85:A:TYR:HE2 | 1:153:A:ILE:H | 3 | 0.51 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 10 | 0.51 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 10 | 0.51 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 10 | 0.51 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 10 | 0.51 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 10 | 0.51 |
| (2,348) | 1:62:A:VAL:HA | 1:175:A:PHE:HD1 | 6 | 0.51 |
| (2,348) | 1:62:A:VAL:HA | 1:175:A:PHE:HD2 | 6 | 0.51 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 2 | 0.51 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 2 | 0.51 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 7 | 0.51 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 7 | 0.51 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 9 | 0.51 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 1 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 2 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 4 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 4 | 0.51 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 4 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 4 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 4 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 4 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 4 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 4 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 4 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 5 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 6 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 7 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 8 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 8 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 8 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 8 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 8 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 8 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 8 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 8 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 8 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 9 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 10 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 10 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 10 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 10 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 10 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 10 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 10 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 10 | 0.51 |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 10 | 0.51 |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H | 5 | 0.51 |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H | 5 | 0.51 |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H | 5 | 0.51 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 10 | 0.51 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 10 | 0.51 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 10 | 0.51 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 2 | 0.51 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 2 | 0.51 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 2 | 0.51 |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA | 6 | 0.51 |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA | 6 | 0.51 |
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA | 6 | 0.51 |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA | 8 | 0.51 |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA | 8 | 0.51 |
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA | 8 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 2 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 2 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 2 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 4 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 4 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 4 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 5 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 5 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 5 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 8 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 8 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 8 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 9 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 9 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 9 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 10 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 10 | 0.51 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 10 | 0.51 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD21 | 7 | 0.51 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD22 | 7 | 0.51 |
| (1,1104) | 1:77:A:LEU:H | 1:104:A:LEU:HD23 | 7 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H | 6 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H | 6 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H | 6 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H | 6 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H | 6 | 0.51 |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H | 6 | 0.51 |
| (1,851) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD11 | 9 | 0.51 |
| (1,851) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD12 | 9 | 0.51 |
| (1,851) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD13 | 9 | 0.51 |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H | 2 | 0.51 |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H | 2 | 0.51 |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H | 2 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 1 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 1 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 1 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 3 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 3 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 3 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 4 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 4 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 4 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 9 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 9 | 0.51 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 9 | 0.51 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 8 | 0.51 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 8 | 0.51 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 8 | 0.51 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG21 | 9 | 0.5 |
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG22 | 9 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (3,8) | 1:111:A:ILE:HA | 1:111:A:ILE:HG23 | 9 | 0.5 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 9 | 0.5 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 9 | 0.5 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 10 | 0.5 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 10 | 0.5 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 6 | 0.5 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 6 | 0.5 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE1 | 4 | 0.5 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE2 | 4 | 0.5 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE1 | 7 | 0.5 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE2 | 7 | 0.5 |
| (2,659) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H | 9 | 0.5 |
| (2,659) | 1:125:A:LYS:HE3 | 1:125:A:LYS:H | 9 | 0.5 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 10 | 0.5 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 10 | 0.5 |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H | 4 | 0.5 |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H | 4 | 0.5 |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H | 9 | 0.5 |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H | 9 | 0.5 |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H | 2 | 0.5 |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H | 2 | 0.5 |
| (2,631) | 1:122:A:TYR:HD1 | 1:124:A:ASP:H | 5 | 0.5 |
| (2,631) | 1:122:A:TYR:HD2 | 1:124:A:ASP:H | 5 | 0.5 |
| (2,631) | 1:122:A:TYR:HD1 | 1:124:A:ASP:H | 10 | 0.5 |
| (2,631) | 1:122:A:TYR:HD2 | 1:124:A:ASP:H | 10 | 0.5 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 7 | 0.5 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 7 | 0.5 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD11 | 5 | 0.5 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD12 | 5 | 0.5 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD13 | 5 | 0.5 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 1 | 0.5 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 1 | 0.5 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 3 | 0.5 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 3 | 0.5 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 1 | 0.5 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 1 | 0.5 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 1 | 0.5 |
| (2,355) | 1:64:A:LEU:H | 1:175:A:PHE:HE1 | 6 | 0.5 |
| (2,355) | 1:64:A:LEU:H | 1:175:A:PHE:HE2 | 6 | 0.5 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 6 | 0.5 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 6 | 0.5 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 2 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 2 | 0.5 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 4 | 0.5 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 4 | 0.5 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 5 | 0.5 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 5 | 0.5 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 10 | 0.5 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 10 | 0.5 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 10 | 0.5 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 10 | 0.5 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 10 | 0.5 |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H | 2 | 0.5 |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H | 2 | 0.5 |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H | 2 | 0.5 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 4 | 0.5 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 4 | 0.5 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 4 | 0.5 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 4 | 0.5 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 4 | 0.5 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 4 | 0.5 |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA | 5 | 0.5 |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA | 5 | 0.5 |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA | 6 | 0.5 |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA | 6 | 0.5 |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA | 10 | 0.5 |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA | 10 | 0.5 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 6 | 0.5 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 6 | 0.5 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 6 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 3 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 3 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 3 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 6 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 6 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 6 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 7 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 7 | 0.5 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 7 | 0.5 |
| (1,1090) | 1:77:A:LEU:HD11 | 1:79:A:ILE:H | 4 | 0.5 |
| (1,1090) | 1:77:A:LEU:HD12 | 1:79:A:ILE:H | 4 | 0.5 |
| (1,1090) | 1:77:A:LEU:HD13 | 1:79:A:ILE:H | 4 | 0.5 |
| (1,1090) | 1:77:A:LEU:HD21 | 1:79:A:ILE:H | 4 | 0.5 |
| (1,1090) | 1:77:A:LEU:HD22 | 1:79:A:ILE:H | 4 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1090) | 1:77:A:LEU:HD23 | 1:79:A:ILE:H | 4 | 0.5 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 6 | 0.5 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 6 | 0.5 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 6 | 0.5 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 6 | 0.5 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 6 | 0.5 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 6 | 0.5 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 5 | 0.5 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 5 | 0.5 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 5 | 0.5 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 5 | 0.5 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 5 | 0.5 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 5 | 0.5 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 5 | 0.5 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 5 | 0.5 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 5 | 0.5 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 7 | 0.5 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 7 | 0.5 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 7 | 0.5 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 6 | 0.5 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 6 | 0.5 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 6 | 0.5 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 4 | 0.5 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 4 | 0.5 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 4 | 0.5 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 3 | 0.5 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 3 | 0.5 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 3 | 0.5 |
| (2,673) | 1:127:A:GLY:H | 1:128:A:TYR:HD1 | 10 | 0.49 |
| (2,673) | 1:127:A:GLY:H | 1:128:A:TYR:HD2 | 10 | 0.49 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG2 | 6 | 0.49 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG3 | 6 | 0.49 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 8 | 0.49 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 8 | 0.49 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE1 | 7 | 0.49 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE2 | 7 | 0.49 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 7 | 0.49 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 7 | 0.49 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 7 | 0.49 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG21 | 9 | 0.49 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG22 | 9 | 0.49 |
| (2,365) | 1:66:A:ASN:HB3 | 1:173:A:VAL:HG23 | 9 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 1 | 0.49 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 1 | 0.49 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 1 | 0.49 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 1 | 0.49 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 8 | 0.49 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 8 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H | 2 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H | 2 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H | 2 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H | 4 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H | 4 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H | 4 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H | 5 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H | 5 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H | 5 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H | 7 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H | 7 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H | 7 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H | 10 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H | 10 | 0.49 |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H | 10 | 0.49 |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA | 3 | 0.49 |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA | 3 | 0.49 |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA | 4 | 0.49 |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA | 4 | 0.49 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 6 | 0.49 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 6 | 0.49 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 6 | 0.49 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 6 | 0.49 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 6 | 0.49 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 6 | 0.49 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 5 | 0.49 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 5 | 0.49 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 5 | 0.49 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 8 | 0.49 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 8 | 0.49 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 8 | 0.49 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG21 | 5 | 0.49 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG22 | 5 | 0.49 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG23 | 5 | 0.49 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 8 | 0.49 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 8 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 8 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1 | 6 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2 | 6 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3 | 6 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1 | 6 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2 | 6 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3 | 6 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1 | 6 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2 | 6 | 0.49 |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3 | 6 | 0.49 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 7 | 0.49 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 7 | 0.49 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 7 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG21 | 8 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG22 | 8 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG23 | 8 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG21 | 8 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG22 | 8 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG23 | 8 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG21 | 8 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG22 | 8 | 0.49 |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG23 | 8 | 0.49 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 6 | 0.49 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 6 | 0.49 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 6 | 0.49 |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H | 1 | 0.49 |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H | 1 | 0.49 |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H | 1 | 0.49 |
| (1,1090) | 1:77:A:LEU:HD11 | 1:79:A:ILE:H | 8 | 0.49 |
| (1,1090) | 1:77:A:LEU:HD12 | 1:79:A:ILE:H | 8 | 0.49 |
| (1,1090) | 1:77:A:LEU:HD13 | 1:79:A:ILE:H | 8 | 0.49 |
| (1,1090) | 1:77:A:LEU:HD21 | 1:79:A:ILE:H | 8 | 0.49 |
| (1,1090) | 1:77:A:LEU:HD22 | 1:79:A:ILE:H | 8 | 0.49 |
| (1,1090) | 1:77:A:LEU:HD23 | 1:79:A:ILE:H | 8 | 0.49 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 3 | 0.49 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 3 | 0.49 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 3 | 0.49 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 1 | 0.49 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 1 | 0.49 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 1 | 0.49 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 1 | 0.49 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 1 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 1 | 0.49 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 3 | 0.49 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 3 | 0.49 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 3 | 0.49 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 5 | 0.49 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 5 | 0.49 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 5 | 0.49 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 9 | 0.49 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 9 | 0.49 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 9 | 0.49 |
| (2,631) | 1:122:A:TYR:HD1 | 1:124:A:ASP:H | 2 | 0.48 |
| (2,631) | 1:122:A:TYR:HD2 | 1:124:A:ASP:H | 2 | 0.48 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 10 | 0.48 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 10 | 0.48 |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H | 9 | 0.48 |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H | 9 | 0.48 |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H | 9 | 0.48 |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA | 8 | 0.48 |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA | 8 | 0.48 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 4 | 0.48 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 4 | 0.48 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 4 | 0.48 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 8 | 0.48 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 8 | 0.48 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 8 | 0.48 |
| (1,1662) | 1:113:A:LEU:HD11 | 1:113:A:LEU:H | 1 | 0.48 |
| (1,1662) | 1:113:A:LEU:HD12 | 1:113:A:LEU:H | 1 | 0.48 |
| (1,1662) | 1:113:A:LEU:HD13 | 1:113:A:LEU:H | 1 | 0.48 |
| (1,1662) | 1:113:A:LEU:HD11 | 1:113:A:LEU:H | 7 | 0.48 |
| (1,1662) | 1:113:A:LEU:HD12 | 1:113:A:LEU:H | 7 | 0.48 |
| (1,1662) | 1:113:A:LEU:HD13 | 1:113:A:LEU:H | 7 | 0.48 |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H | 2 | 0.48 |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H | 2 | 0.48 |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H | 2 | 0.48 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 2 | 0.48 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 2 | 0.48 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 2 | 0.48 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 10 | 0.48 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 10 | 0.48 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 10 | 0.48 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG21 | 5 | 0.48 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG22 | 5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG23 | 5 | 0.48 |
| (1,289) | 1:37:A:GLY:HA3 | 1:37:A:GLY:H | 2 | 0.48 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 2 | 0.48 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 2 | 0.48 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 2 | 0.48 |
| (1,126) | 1:27:A:SER:HB2 | 1:177:A:PHE:HE1 | 10 | 0.48 |
| (1,126) | 1:27:A:SER:HB2 | 1:177:A:PHE:HE2 | 10 | 0.48 |
| (1,126) | 1:27:A:SER:HB3 | 1:177:A:PHE:HE1 | 10 | 0.48 |
| (1,126) | 1:27:A:SER:HB3 | 1:177:A:PHE:HE2 | 10 | 0.48 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 2 | 0.47 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 2 | 0.47 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 10 | 0.47 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 10 | 0.47 |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H | 3 | 0.47 |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H | 3 | 0.47 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 5 | 0.47 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 5 | 0.47 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 7 | 0.47 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 7 | 0.47 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE1 | 1 | 0.47 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE2 | 1 | 0.47 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 6 | 0.47 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 6 | 0.47 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 6 | 0.47 |
| (2,240) | 1:46:A:TYR:HB2 | 1:155:A:ASN:HD21 | 1 | 0.47 |
| (2,240) | 1:46:A:TYR:HB2 | 1:155:A:ASN:HD22 | 1 | 0.47 |
| (2,94) | 1:23:A:ILE:HD11 | 1:53:A:ASP:H | 9 | 0.47 |
| (2,94) | 1:23:A:ILE:HD12 | 1:53:A:ASP:H | 9 | 0.47 |
| (2,94) | 1:23:A:ILE:HD13 | 1:53:A:ASP:H | 9 | 0.47 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 7 | 0.47 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 7 | 0.47 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 7 | 0.47 |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H | 3 | 0.47 |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H | 3 | 0.47 |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H | 3 | 0.47 |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H | 1 | 0.47 |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H | 1 | 0.47 |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H | 1 | 0.47 |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H | 7 | 0.47 |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H | 7 | 0.47 |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H | 7 | 0.47 |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA | 1 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA | 1 | 0.47 |
| (1,2081) | 1:151:A:VAL:HG11 | 1:153:A:ILE:H | 6 | 0.47 |
| (1,2081) | 1:151:A:VAL:HG12 | 1:153:A:ILE:H | 6 | 0.47 |
| (1,2081) | 1:151:A:VAL:HG13 | 1:153:A:ILE:H | 6 | 0.47 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 3 | 0.47 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 3 | 0.47 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 3 | 0.47 |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB | 10 | 0.47 |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB | 10 | 0.47 |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB | 10 | 0.47 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 8 | 0.47 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 8 | 0.47 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 8 | 0.47 |
| (1,1758) | 1:119:A:ALA:HB1 | 1:151:A:VAL:H | 9 | 0.47 |
| (1,1758) | 1:119:A:ALA:HB2 | 1:151:A:VAL:H | 9 | 0.47 |
| (1,1758) | 1:119:A:ALA:HB3 | 1:151:A:VAL:H | 9 | 0.47 |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H | 1 | 0.47 |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H | 1 | 0.47 |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H | 1 | 0.47 |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H | 10 | 0.47 |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H | 10 | 0.47 |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H | 10 | 0.47 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 3 | 0.47 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 3 | 0.47 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 3 | 0.47 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 9 | 0.47 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 9 | 0.47 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 9 | 0.47 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 1 | 0.47 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 1 | 0.47 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 1 | 0.47 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 4 | 0.47 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 4 | 0.47 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 4 | 0.47 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 8 | 0.47 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 8 | 0.47 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 8 | 0.47 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 9 | 0.47 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 9 | 0.47 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 9 | 0.47 |
| (1,1475) | 1:95:A:PHE:HB2 | 1:96:A:SER:H | 2 | 0.47 |
| (1,1475) | 1:95:A:PHE:HB3 | 1:96:A:SER:H | 2 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1460) | 1:92:A:LEU:HG | 1:93:A:GLY:H | 8 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3 | 9 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3 | 9 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3 | 9 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3 | 9 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3 | 9 | 0.47 |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3 | 9 | 0.47 |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H | 5 | 0.47 |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H | 5 | 0.47 |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H | 5 | 0.47 |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H | 5 | 0.47 |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H | 5 | 0.47 |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H | 5 | 0.47 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 9 | 0.47 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 9 | 0.47 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 9 | 0.47 |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H | 9 | 0.47 |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H | 9 | 0.47 |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H | 9 | 0.47 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 2 | 0.47 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 2 | 0.47 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 2 | 0.47 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 3 | 0.47 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 3 | 0.47 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 3 | 0.47 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 8 | 0.47 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 8 | 0.47 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 8 | 0.47 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 9 | 0.47 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 9 | 0.47 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 9 | 0.47 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 10 | 0.47 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 10 | 0.47 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 10 | 0.47 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 2 | 0.47 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 2 | 0.47 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 2 | 0.47 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 3 | 0.47 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 3 | 0.47 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 3 | 0.47 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 8 | 0.47 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 8 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 8 | 0.47 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 9 | 0.47 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 9 | 0.47 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 9 | 0.47 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 10 | 0.47 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 10 | 0.47 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 10 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 1 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 1 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 1 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 2 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 2 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 2 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 3 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 3 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 3 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 6 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 6 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 6 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 7 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 7 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 7 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 8 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 8 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 8 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 10 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 10 | 0.47 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 10 | 0.47 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 7 | 0.47 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 7 | 0.47 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 7 | 0.47 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE1 | 9 | 0.47 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE2 | 9 | 0.47 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE1 | 9 | 0.47 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE2 | 9 | 0.47 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE1 | 9 | 0.47 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE2 | 9 | 0.47 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 6 | 0.47 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 6 | 0.47 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 6 | 0.47 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 2 | 0.47 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 2 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 2 | 0.47 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 4 | 0.47 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 4 | 0.47 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 4 | 0.47 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 3 | 0.46 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 3 | 0.46 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 5 | 0.46 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 5 | 0.46 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 5 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 8 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 8 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 8 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 8 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 8 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 8 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 8 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 8 | 0.46 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 8 | 0.46 |
| (1,2176) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HE1 | 10 | 0.46 |
| (1,2176) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HE2 | 10 | 0.46 |
| (1,2176) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HE1 | 10 | 0.46 |
| (1,2176) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HE2 | 10 | 0.46 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 5 | 0.46 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 5 | 0.46 |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 5 | 0.46 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 7 | 0.46 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 7 | 0.46 |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 7 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 1 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 1 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 1 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 2 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 2 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 2 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 3 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 3 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 3 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 4 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 4 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 4 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 5 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 5 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 5 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 6 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 6 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 6 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 7 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 7 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 7 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 9 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 9 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 9 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG21 | 10 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 10 | 0.46 |
| (1,1804) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 10 | 0.46 |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H | 5 | 0.46 |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H | 5 | 0.46 |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H | 5 | 0.46 |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H | 7 | 0.46 |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H | 7 | 0.46 |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H | 7 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 2 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 2 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 2 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 4 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 4 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 4 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 5 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 5 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 5 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 7 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 7 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 7 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 10 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 10 | 0.46 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 10 | 0.46 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 10 | 0.46 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 10 | 0.46 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 10 | 0.46 |
| (1,1545) | 1:102:A:ILE:HG21 | 1:107:A:PRO:HA | 4 | 0.46 |
| (1,1545) | 1:102:A:ILE:HG22 | 1:107:A:PRO:HA | 4 | 0.46 |
| (1,1545) | 1:102:A:ILE:HG23 | 1:107:A:PRO:HA | 4 | 0.46 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 5 | 0.46 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 5 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 3 | 0.46 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 3 | 0.46 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 3 | 0.46 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 4 | 0.46 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 4 | 0.46 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 4 | 0.46 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG11 | 1 | 0.46 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG12 | 1 | 0.46 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG13 | 1 | 0.46 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 7 | 0.46 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 7 | 0.46 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 7 | 0.46 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 7 | 0.46 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 7 | 0.46 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 7 | 0.46 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 4 | 0.46 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 4 | 0.46 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 4 | 0.46 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB1 | 5 | 0.46 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB2 | 5 | 0.46 |
| (1,294) | 1:38:A:ALA:HA | 1:38:A:ALA:HB3 | 5 | 0.46 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 2 | 0.46 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 2 | 0.46 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 2 | 0.46 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 2 | 0.46 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 2 | 0.46 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 2 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 1 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 1 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 1 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 2 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 2 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 2 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 3 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 3 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 3 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 4 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 4 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 4 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 5 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 5 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 5 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 6 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 6 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 6 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 7 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 7 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 7 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 8 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 8 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 8 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 9 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 9 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 9 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG21 | 10 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG22 | 10 | 0.46 |
| (1,1) | 1:15:A:THR:HB | 1:15:A:THR:HG23 | 10 | 0.46 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 2 | 0.45 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 2 | 0.45 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 2 | 0.45 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 2 | 0.45 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 8 | 0.45 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 8 | 0.45 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 8 | 0.45 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 1 | 0.45 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 1 | 0.45 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 1 | 0.45 |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H | 3 | 0.45 |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H | 3 | 0.45 |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H | 3 | 0.45 |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H | 8 | 0.45 |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H | 8 | 0.45 |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H | 8 | 0.45 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 3 | 0.45 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 3 | 0.45 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 3 | 0.45 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 10 | 0.45 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 10 | 0.45 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 10 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 1 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 1 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 1 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 4 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 4 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 4 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 9 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 9 | 0.45 |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 9 | 0.45 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 10 | 0.45 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 10 | 0.45 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 10 | 0.45 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 3 | 0.45 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 3 | 0.45 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 3 | 0.45 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG21 | 1 | 0.45 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG22 | 1 | 0.45 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG23 | 1 | 0.45 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG21 | 4 | 0.45 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG22 | 4 | 0.45 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG23 | 4 | 0.45 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG21 | 10 | 0.45 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG22 | 10 | 0.45 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG23 | 10 | 0.45 |
| (1,1766) | 1:120:A:VAL:HG11 | 1:120:A:VAL:H | 4 | 0.45 |
| (1,1766) | 1:120:A:VAL:HG12 | 1:120:A:VAL:H | 4 | 0.45 |
| (1,1766) | 1:120:A:VAL:HG13 | 1:120:A:VAL:H | 4 | 0.45 |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H | 8 | 0.45 |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H | 8 | 0.45 |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H | 8 | 0.45 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 6 | 0.45 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 6 | 0.45 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 6 | 0.45 |
| (1,1338) | 1:85:A:TYR:HD1 | 1:86:A:GLU:H | 5 | 0.45 |
| (1,1338) | 1:85:A:TYR:HD2 | 1:86:A:GLU:H | 5 | 0.45 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 8 | 0.45 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 8 | 0.45 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 8 | 0.45 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 2 | 0.45 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 2 | 0.45 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 2 | 0.45 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 4 | 0.45 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 4 | 0.45 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 4 | 0.45 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 5 | 0.45 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 5 | 0.45 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 5 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 7 | 0.45 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 7 | 0.45 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 7 | 0.45 |
| (1,947) | 1:71:A:LYS:HG3 | 1:71:A:LYS:H | 5 | 0.45 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 1 | 0.45 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 1 | 0.45 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 1 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 1 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 1 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 1 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 2 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 2 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 2 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 3 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 3 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 3 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 4 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 4 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 4 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 5 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 5 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 5 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 6 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 6 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 6 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 7 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 7 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 7 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 8 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 8 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 8 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD11 | 10 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD12 | 10 | 0.45 |
| (1,840) | 1:66:A:ASN:HB2 | 1:174:A:ILE:HD13 | 10 | 0.45 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 3 | 0.45 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 3 | 0.45 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 3 | 0.45 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 3 | 0.45 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 3 | 0.45 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 3 | 0.45 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 4 | 0.45 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 4 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 4 | 0.45 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 4 | 0.45 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 4 | 0.45 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 4 | 0.45 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 7 | 0.45 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 7 | 0.45 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 7 | 0.45 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 5 | 0.45 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 5 | 0.45 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 5 | 0.45 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 5 | 0.45 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 4 | 0.45 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 4 | 0.45 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 4 | 0.44 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 4 | 0.44 |
| (2,689) | 1:131:A:THR:HA | 1:145:A:TYR:HD1 | 1 | 0.44 |
| (2,689) | 1:131:A:THR:HA | 1:145:A:TYR:HD2 | 1 | 0.44 |
| (2,689) | 1:131:A:THR:HA | 1:145:A:TYR:HD1 | 4 | 0.44 |
| (2,689) | 1:131:A:THR:HA | 1:145:A:TYR:HD2 | 4 | 0.44 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 1 | 0.44 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 1 | 0.44 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 8 | 0.44 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 8 | 0.44 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 2 | 0.44 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 2 | 0.44 |
| (2,454) | 1:78:A:GLN:HE21 | 1:101:A:VAL:HG11 | 3 | 0.44 |
| (2,454) | 1:78:A:GLN:HE21 | 1:101:A:VAL:HG12 | 3 | 0.44 |
| (2,454) | 1:78:A:GLN:HE21 | 1:101:A:VAL:HG13 | 3 | 0.44 |
| (2,295) | 1:52:A:LYS:HE2 | 1:54:A:GLN:HE22 | 4 | 0.44 |
| (2,295) | 1:52:A:LYS:HE3 | 1:54:A:GLN:HE22 | 4 | 0.44 |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H | 4 | 0.44 |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H | 4 | 0.44 |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H | 4 | 0.44 |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H | 5 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H | 5 | 0.44 |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H | 5 | 0.44 |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H | 6 | 0.44 |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H | 6 | 0.44 |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H | 6 | 0.44 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 5 | 0.44 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 5 | 0.44 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 5 | 0.44 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 3 | 0.44 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 3 | 0.44 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 3 | 0.44 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 3 | 0.44 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 3 | 0.44 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 3 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 2 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 2 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 2 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 3 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 3 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 3 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H | 8 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H | 8 | 0.44 |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H | 8 | 0.44 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 7 | 0.44 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 7 | 0.44 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 7 | 0.44 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG21 | 8 | 0.44 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG22 | 8 | 0.44 |
| (1,1840) | 1:132:A:SER:HB3 | 1:142:A:ILE:HG23 | 8 | 0.44 |
| (1,1766) | 1:120:A:VAL:HG11 | 1:120:A:VAL:H | 7 | 0.44 |
| (1,1766) | 1:120:A:VAL:HG12 | 1:120:A:VAL:H | 7 | 0.44 |
| (1,1766) | 1:120:A:VAL:HG13 | 1:120:A:VAL:H | 7 | 0.44 |
| (1,1766) | 1:120:A:VAL:HG11 | 1:120:A:VAL:H | 10 | 0.44 |
| (1,1766) | 1:120:A:VAL:HG12 | 1:120:A:VAL:H | 10 | 0.44 |
| (1,1766) | 1:120:A:VAL:HG13 | 1:120:A:VAL:H | 10 | 0.44 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 8 | 0.44 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 8 | 0.44 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 8 | 0.44 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 4 | 0.44 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 4 | 0.44 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 8 | 0.44 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 8 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 8 | 0.44 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 10 | 0.44 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 10 | 0.44 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 10 | 0.44 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 5 | 0.44 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 5 | 0.44 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 5 | 0.44 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 5 | 0.44 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 5 | 0.44 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 5 | 0.44 |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H | 3 | 0.44 |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H | 3 | 0.44 |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H | 3 | 0.44 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB1 | 1 | 0.44 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB2 | 1 | 0.44 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB3 | 1 | 0.44 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB1 | 1 | 0.44 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB2 | 1 | 0.44 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB3 | 1 | 0.44 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 5 | 0.44 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 5 | 0.44 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 5 | 0.44 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 5 | 0.44 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 5 | 0.44 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 5 | 0.44 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 9 | 0.44 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 9 | 0.44 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 9 | 0.44 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 9 | 0.44 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 9 | 0.44 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 9 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 1 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 2 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 2 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 2 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 2 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 2 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 2 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 2 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 2 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 2 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 7 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 7 | 0.44 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 7 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 7 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 7 | 0.44 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 7 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 7 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 7 | 0.44 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 7 | 0.44 |
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG21 | 10 | 0.44 |
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG22 | 10 | 0.44 |
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG23 | 10 | 0.44 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG21 | 10 | 0.44 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG22 | 10 | 0.44 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG23 | 10 | 0.44 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG21 | 10 | 0.44 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG22 | 10 | 0.44 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG23 | 10 | 0.44 |
| (1,6) | 1:18:A:ALA:HB1 | 1:19:A:VAL:H | 7 | 0.44 |
| (1,6) | 1:18:A:ALA:HB2 | 1:19:A:VAL:H | 7 | 0.44 |
| (1,6) | 1:18:A:ALA:HB3 | 1:19:A:VAL:H | 7 | 0.44 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 7 | 0.43 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 7 | 0.43 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 7 | 0.43 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 7 | 0.43 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 7 | 0.43 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 7 | 0.43 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE1 | 9 | 0.43 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE2 | 9 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 4 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 4 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 4 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 4 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 4 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 4 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 4 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 4 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 4 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 5 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 5 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 5 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 5 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 5 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 5 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 5 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 5 | 0.43 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 5 | 0.43 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 3 | 0.43 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 3 | 0.43 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 8 | 0.43 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 8 | 0.43 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 1 | 0.43 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 1 | 0.43 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 1 | 0.43 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 5 | 0.43 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 5 | 0.43 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 5 | 0.43 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG21 | 6 | 0.43 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG22 | 6 | 0.43 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG23 | 6 | 0.43 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG21 | 6 | 0.43 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG22 | 6 | 0.43 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG23 | 6 | 0.43 |
| (1,1337) | 1:85:A:TYR:HD1 | 1:85:A:TYR:H | 2 | 0.43 |
| (1,1337) | 1:85:A:TYR:HD2 | 1:85:A:TYR:H | 2 | 0.43 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 9 | 0.43 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 9 | 0.43 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 9 | 0.43 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 9 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG21 | 7 | 0.43 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG22 | 7 | 0.43 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG23 | 7 | 0.43 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 7 | 0.43 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 7 | 0.43 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 7 | 0.43 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB1 | 9 | 0.43 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB2 | 9 | 0.43 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB3 | 9 | 0.43 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB1 | 9 | 0.43 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB2 | 9 | 0.43 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB3 | 9 | 0.43 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 5 | 0.43 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 5 | 0.43 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 5 | 0.43 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 9 | 0.43 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 9 | 0.43 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 9 | 0.43 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 9 | 0.43 |
| (1,11) | 1:20:A:SER:HB2 | 1:21:A:GLU:H | 10 | 0.43 |
| (1,11) | 1:20:A:SER:HB3 | 1:21:A:GLU:H | 10 | 0.43 |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA | 5 | 0.42 |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA | 5 | 0.42 |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA | 5 | 0.42 |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 2 | 0.42 |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 2 | 0.42 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 2 | 0.42 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 10 | 0.42 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 10 | 0.42 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 10 | 0.42 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 10 | 0.42 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 10 | 0.42 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 10 | 0.42 |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1 | 8 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2 | 8 | 0.42 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 1 | 0.42 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 1 | 0.42 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 1 | 0.42 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 1 | 0.42 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 1 | 0.42 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 1 | 0.42 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 6 | 0.42 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 6 | 0.42 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 6 | 0.42 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 9 | 0.42 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 9 | 0.42 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 9 | 0.42 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 1 | 0.42 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 1 | 0.42 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 1 | 0.42 |
| (1,2080) | 1:151:A:VAL:HG11 | 1:152:A:ALA:H | 10 | 0.42 |
| (1,2080) | 1:151:A:VAL:HG12 | 1:152:A:ALA:H | 10 | 0.42 |
| (1,2080) | 1:151:A:VAL:HG13 | 1:152:A:ALA:H | 10 | 0.42 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 6 | 0.42 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 6 | 0.42 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD21 | 9 | 0.42 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD22 | 9 | 0.42 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 4 | 0.42 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 4 | 0.42 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 4 | 0.42 |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H | 10 | 0.42 |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H | 10 | 0.42 |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H | 10 | 0.42 |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H | 10 | 0.42 |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H | 10 | 0.42 |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 3 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 4 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 4 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 4 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 4 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 4 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 4 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 4 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 4 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 4 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 10 | 0.42 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 10 | 0.42 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD11 | 1 | 0.42 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD12 | 1 | 0.42 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD13 | 1 | 0.42 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD11 | 2 | 0.42 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD12 | 2 | 0.42 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD13 | 2 | 0.42 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 10 | 0.42 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 10 | 0.42 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 10 | 0.42 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 2 | 0.41 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 2 | 0.41 |
| (2,601) | 1:115:A:LYS:HE2 | 1:116:A:GLU:H | 6 | 0.41 |
| (2,601) | 1:115:A:LYS:HE3 | 1:116:A:GLU:H | 6 | 0.41 |
| (2,240) | 1:46:A:TYR:HB2 | 1:155:A:ASN:HD21 | 5 | 0.41 |
| (2,240) | 1:46:A:TYR:HB2 | 1:155:A:ASN:HD22 | 5 | 0.41 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 4 | 0.41 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 4 | 0.41 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 4 | 0.41 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 3 | 0.41 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 3 | 0.41 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 3 | 0.41 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 6 | 0.41 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 6 | 0.41 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 6 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 1 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 1 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 1 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 3 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 3 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 3 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 7 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 7 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 7 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 10 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 10 | 0.41 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 10 | 0.41 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 10 | 0.41 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 10 | 0.41 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 10 | 0.41 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 4 | 0.41 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 4 | 0.41 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 4 | 0.41 |
| (1,2081) | 1:151:A:VAL:HG11 | 1:153:A:ILE:H | 10 | 0.41 |
| (1,2081) | 1:151:A:VAL:HG12 | 1:153:A:ILE:H | 10 | 0.41 |
| (1,2081) | 1:151:A:VAL:HG13 | 1:153:A:ILE:H | 10 | 0.41 |
| (1,2080) | 1:151:A:VAL:HG11 | 1:152:A:ALA:H | 6 | 0.41 |
| (1,2080) | 1:151:A:VAL:HG12 | 1:152:A:ALA:H | 6 | 0.41 |
| (1,2080) | 1:151:A:VAL:HG13 | 1:152:A:ALA:H | 6 | 0.41 |
| (1,1801) | 1:128:A:TYR:HD1 | 1:131:A:THR:HG21 | 8 | 0.41 |
| (1,1801) | 1:128:A:TYR:HD1 | 1:131:A:THR:HG22 | 8 | 0.41 |
| (1,1801) | 1:128:A:TYR:HD1 | 1:131:A:THR:HG23 | 8 | 0.41 |
| (1,1801) | 1:128:A:TYR:HD2 | 1:131:A:THR:HG21 | 8 | 0.41 |
| (1,1801) | 1:128:A:TYR:HD2 | 1:131:A:THR:HG22 | 8 | 0.41 |
| (1,1801) | 1:128:A:TYR:HD2 | 1:131:A:THR:HG23 | 8 | 0.41 |
| (1,1475) | 1:95:A:PHE:HB2 | 1:96:A:SER:H | 5 | 0.41 |
| (1,1475) | 1:95:A:PHE:HB3 | 1:96:A:SER:H | 5 | 0.41 |
| (1,1275) | 1:82:A:THR:HG21 | 1:96:A:SER:HB2 | 9 | 0.41 |
| (1,1275) | 1:82:A:THR:HG22 | 1:96:A:SER:HB2 | 9 | 0.41 |
| (1,1275) | 1:82:A:THR:HG23 | 1:96:A:SER:HB2 | 9 | 0.41 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 1 | 0.41 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 1 | 0.41 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 1 | 0.41 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 3 | 0.41 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 3 | 0.41 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 3 | 0.41 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 6 | 0.41 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 6 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 6 | 0.41 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 10 | 0.41 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 10 | 0.41 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 10 | 0.41 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 2 | 0.41 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 6 | 0.41 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 6 | 0.41 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 6 | 0.41 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 9 | 0.41 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 9 | 0.41 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 9 | 0.41 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD11 | 1 | 0.41 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD12 | 1 | 0.41 |
| (1,205) | 1:32:A:ILE:HA | 1:32:A:ILE:HD13 | 1 | 0.41 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 6 | 0.41 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 8 | 0.41 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 8 | 0.41 |
| (1,162) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 8 | 0.41 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 8 | 0.41 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 8 | 0.41 |
| (1,162) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 8 | 0.41 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 8 | 0.41 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 8 | 0.41 |
| (1,162) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 8 | 0.41 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD11 | 9 | 0.41 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD12 | 9 | 0.41 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD13 | 9 | 0.41 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 6 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 6 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 6 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 8 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 8 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 8 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 9 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 9 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 9 | 0.4 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 6 | 0.4 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 6 | 0.4 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 6 | 0.4 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 8 | 0.4 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 8 | 0.4 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 8 | 0.4 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 9 | 0.4 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 9 | 0.4 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 9 | 0.4 |
| (2,661) | 1:125:A:LYS:HG2 | 1:126:A:THR:H | 10 | 0.4 |
| (2,661) | 1:125:A:LYS:HG3 | 1:126:A:THR:H | 10 | 0.4 |
| (2,295) | 1:52:A:LYS:HE2 | 1:54:A:GLN:HE22 | 2 | 0.4 |
| (2,295) | 1:52:A:LYS:HE3 | 1:54:A:GLN:HE22 | 2 | 0.4 |
| (2,227) | 1:43:A:ASP:HB3 | 1:46:A:TYR:HE1 | 8 | 0.4 |
| (2,227) | 1:43:A:ASP:HB3 | 1:46:A:TYR:HE2 | 8 | 0.4 |
| (2,16) | 1:17:A:GLN:HG2 | 1:18:A:ALA:H | 6 | 0.4 |
| (2,16) | 1:17:A:GLN:HG3 | 1:18:A:ALA:H | 6 | 0.4 |
| (1,2327) | 1:171:A:LEU:HG | 1:171:A:LEU:H | 2 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 3 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 3 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 3 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 3 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 3 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 3 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 3 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 3 | 0.4 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 3 | 0.4 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD11 | 7 | 0.4 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD12 | 7 | 0.4 |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD13 | 7 | 0.4 |
| (1,2191) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HE1 | 10 | 0.4 |
| (1,2191) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HE2 | 10 | 0.4 |
| (1,2191) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HE1 | 10 | 0.4 |
| (1,2191) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HE2 | 10 | 0.4 |
| (1,2191) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HE1 | 10 | 0.4 |
| (1,2191) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HE2 | 10 | 0.4 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 8 | 0.4 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 8 | 0.4 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 8 | 0.4 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 1 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 1 | 0.4 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 1 | 0.4 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD21 | 4 | 0.4 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD22 | 4 | 0.4 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 4 | 0.4 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 4 | 0.4 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 4 | 0.4 |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H | 8 | 0.4 |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H | 8 | 0.4 |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H | 8 | 0.4 |
| (1,1475) | 1:95:A:PHE:HB2 | 1:96:A:SER:H | 1 | 0.4 |
| (1,1475) | 1:95:A:PHE:HB3 | 1:96:A:SER:H | 1 | 0.4 |
| (1,1475) | 1:95:A:PHE:HB2 | 1:96:A:SER:H | 9 | 0.4 |
| (1,1475) | 1:95:A:PHE:HB3 | 1:96:A:SER:H | 9 | 0.4 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 9 | 0.4 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 9 | 0.4 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 9 | 0.4 |
| (1,1339) | 1:85:A:TYR:HD1 | 1:135:A:VAL:HA | 5 | 0.4 |
| (1,1339) | 1:85:A:TYR:HD2 | 1:135:A:VAL:HA | 5 | 0.4 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 7 | 0.4 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 7 | 0.4 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 7 | 0.4 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 1 | 0.4 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 1 | 0.4 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 1 | 0.4 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD21 | 7 | 0.4 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD22 | 7 | 0.4 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD23 | 7 | 0.4 |
| (1,605) | 1:54:A:GLN:HG2 | 1:54:A:GLN:H | 5 | 0.4 |
| (1,605) | 1:54:A:GLN:HG3 | 1:54:A:GLN:H | 5 | 0.4 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 10 | 0.4 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 10 | 0.4 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 10 | 0.4 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 3 | 0.4 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 3 | 0.4 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 3 | 0.4 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 6 | 0.4 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE1 | 2 | 0.4 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE2 | 2 | 0.4 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 6 | 0.4 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 6 | 0.4 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 6 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 6 | 0.4 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 6 | 0.4 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 6 | 0.4 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 7 | 0.4 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 7 | 0.4 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 7 | 0.4 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 7 | 0.4 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 7 | 0.4 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 7 | 0.4 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 1 | 0.4 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 1 | 0.4 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 1 | 0.4 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 1 | 0.4 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 1 | 0.4 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 1 | 0.4 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 1 | 0.4 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 1 | 0.4 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 1 | 0.4 |
| (1,166) | 1:29:A:LEU:HD11 | 1:175:A:PHE:H | 6 | 0.4 |
| (1,166) | 1:29:A:LEU:HD12 | 1:175:A:PHE:H | 6 | 0.4 |
| (1,166) | 1:29:A:LEU:HD13 | 1:175:A:PHE:H | 6 | 0.4 |
| (1,11) | 1:20:A:SER:HB2 | 1:21:A:GLU:H | 5 | 0.4 |
| (1,11) | 1:20:A:SER:HB3 | 1:21:A:GLU:H | 5 | 0.4 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 5 | 0.39 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 5 | 0.39 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 5 | 0.39 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 8 | 0.39 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 8 | 0.39 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 8 | 0.39 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 5 | 0.39 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 5 | 0.39 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 5 | 0.39 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 8 | 0.39 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 8 | 0.39 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 8 | 0.39 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE1 | 6 | 0.39 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE2 | 6 | 0.39 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 6 | 0.39 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 6 | 0.39 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 6 | 0.39 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 4 | 0.39 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 4 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 4 | 0.39 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 9 | 0.39 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 9 | 0.39 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 9 | 0.39 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 9 | 0.39 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 9 | 0.39 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 9 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 2 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 2 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 2 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 2 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 2 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 2 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 2 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 2 | 0.39 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 2 | 0.39 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 5 | 0.39 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 5 | 0.39 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 5 | 0.39 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 9 | 0.39 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 9 | 0.39 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 9 | 0.39 |
| (1,2002) | 1:142:A:ILE:HA | 1:142:A:ILE:HD11 | 1 | 0.39 |
| (1,2002) | 1:142:A:ILE:HA | 1:142:A:ILE:HD12 | 1 | 0.39 |
| (1,2002) | 1:142:A:ILE:HA | 1:142:A:ILE:HD13 | 1 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 5 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 5 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 7 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 7 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 9 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 9 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 10 | 0.39 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 10 | 0.39 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD21 | 10 | 0.39 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD22 | 10 | 0.39 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 9 | 0.39 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 9 | 0.39 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 9 | 0.39 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 6 | 0.39 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 6 | 0.39 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 6 | 0.39 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD11 | 4 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD12 | 4 | 0.39 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD13 | 4 | 0.39 |
| (1,1475) | 1:95:A:PHE:HB2 | 1:96:A:SER:H | 8 | 0.39 |
| (1,1475) | 1:95:A:PHE:HB3 | 1:96:A:SER:H | 8 | 0.39 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 2 | 0.39 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 2 | 0.39 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 2 | 0.39 |
| (1,1338) | 1:85:A:TYR:HD1 | 1:86:A:GLU:H | 1 | 0.39 |
| (1,1338) | 1:85:A:TYR:HD2 | 1:86:A:GLU:H | 1 | 0.39 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 5 | 0.39 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 5 | 0.39 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 5 | 0.39 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 9 | 0.39 |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 9 | 0.39 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 9 | 0.39 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 4 | 0.39 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 4 | 0.39 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 4 | 0.39 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 9 | 0.39 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 9 | 0.39 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 9 | 0.39 |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA | 2 | 0.39 |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA | 2 | 0.39 |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA | 2 | 0.39 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG21 | 2 | 0.39 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG22 | 2 | 0.39 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG23 | 2 | 0.39 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG21 | 2 | 0.39 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG22 | 2 | 0.39 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG23 | 2 | 0.39 |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3 | 8 | 0.39 |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3 | 8 | 0.39 |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3 | 8 | 0.39 |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3 | 8 | 0.39 |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3 | 8 | 0.39 |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3 | 8 | 0.39 |
| (1,1091) | 1:77:A:LEU:HD11 | 1:103:A:SER:HA | 8 | 0.39 |
| (1,1091) | 1:77:A:LEU:HD12 | 1:103:A:SER:HA | 8 | 0.39 |
| (1,1091) | 1:77:A:LEU:HD13 | 1:103:A:SER:HA | 8 | 0.39 |
| (1,1091) | 1:77:A:LEU:HD21 | 1:103:A:SER:HA | 8 | 0.39 |
| (1,1091) | 1:77:A:LEU:HD22 | 1:103:A:SER:HA | 8 | 0.39 |
| (1,1091) | 1:77:A:LEU:HD23 | 1:103:A:SER:HA | 8 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 2 | 0.39 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 2 | 0.39 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 2 | 0.39 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 2 | 0.39 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 2 | 0.39 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 2 | 0.39 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 10 | 0.39 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 10 | 0.39 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 10 | 0.39 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 10 | 0.39 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 10 | 0.39 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 10 | 0.39 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG11 | 3 | 0.39 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG12 | 3 | 0.39 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG13 | 3 | 0.39 |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H | 1 | 0.39 |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H | 1 | 0.39 |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H | 1 | 0.39 |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 6 | 0.39 |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 6 | 0.39 |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 6 | 0.39 |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H | 6 | 0.39 |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H | 6 | 0.39 |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H | 6 | 0.39 |
| (1,485) | 1:48:A:ILE:HG13 | 1:48:A:ILE:HG21 | 5 | 0.39 |
| (1,485) | 1:48:A:ILE:HG13 | 1:48:A:ILE:HG22 | 5 | 0.39 |
| (1,485) | 1:48:A:ILE:HG13 | 1:48:A:ILE:HG23 | 5 | 0.39 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 7 | 0.39 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 7 | 0.39 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 7 | 0.39 |
| (1,289) | 1:37:A:GLY:HA3 | 1:37:A:GLY:H | 3 | 0.39 |
| (1,289) | 1:37:A:GLY:HA3 | 1:37:A:GLY:H | 9 | 0.39 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 5 | 0.39 |
| (1,260) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD3 | 2 | 0.39 |
| (1,260) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD3 | 2 | 0.39 |
| (1,260) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD3 | 2 | 0.39 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 6 | 0.39 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 6 | 0.39 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 6 | 0.39 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD11 | 7 | 0.39 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD12 | 7 | 0.39 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD13 | 7 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD11 | 8 | 0.39 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD12 | 8 | 0.39 |
| (1,23) | 1:23:A:ILE:HA | 1:23:A:ILE:HD13 | 8 | 0.39 |
| (1,11) | 1:20:A:SER:HB2 | 1:21:A:GLU:H | 8 | 0.39 |
| (1,11) | 1:20:A:SER:HB3 | 1:21:A:GLU:H | 8 | 0.39 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 6 | 0.39 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 6 | 0.39 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 6 | 0.39 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 3 | 0.38 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 3 | 0.38 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 3 | 0.38 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 3 | 0.38 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 3 | 0.38 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 3 | 0.38 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD11 | 2 | 0.38 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD12 | 2 | 0.38 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD13 | 2 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 1 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 1 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 1 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 2 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 2 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 2 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 4 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 4 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 4 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 5 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 5 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 5 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 7 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 7 | 0.38 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 7 | 0.38 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 7 | 0.38 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 7 | 0.38 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 7 | 0.38 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 8 | 0.38 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 8 | 0.38 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 8 | 0.38 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 6 | 0.38 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 6 | 0.38 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 6 | 0.38 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD21 | 1 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD22 | 1 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 1 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 1 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 1 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 2 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 2 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 2 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 5 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 5 | 0.38 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 5 | 0.38 |
| (1,1695) | 1:115:A:LYS:HA | 1:118:A:ILE:HD11 | 9 | 0.38 |
| (1,1695) | 1:115:A:LYS:HA | 1:118:A:ILE:HD12 | 9 | 0.38 |
| (1,1695) | 1:115:A:LYS:HA | 1:118:A:ILE:HD13 | 9 | 0.38 |
| (1,1475) | 1:95:A:PHE:HB2 | 1:96:A:SER:H | 4 | 0.38 |
| (1,1475) | 1:95:A:PHE:HB3 | 1:96:A:SER:H | 4 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 1 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 1 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 1 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 4 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 4 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 4 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 5 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 5 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 5 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 8 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 8 | 0.38 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 8 | 0.38 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 10 | 0.38 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 10 | 0.38 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 10 | 0.38 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 4 | 0.38 |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H | 7 | 0.38 |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H | 7 | 0.38 |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H | 7 | 0.38 |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H | 7 | 0.38 |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H | 7 | 0.38 |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H | 7 | 0.38 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 6 | 0.38 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 7 | 0.38 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 2 | 0.38 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 2 | 0.38 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 2 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 9 | 0.38 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 9 | 0.38 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 9 | 0.38 |
| (1,269) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HD1 | 2 | 0.38 |
| (1,269) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HD2 | 2 | 0.38 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 10 | 0.38 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 10 | 0.38 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 10 | 0.38 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 10 | 0.38 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 10 | 0.38 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 10 | 0.38 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 10 | 0.38 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 10 | 0.38 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 10 | 0.38 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 2 | 0.38 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 2 | 0.38 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 2 | 0.38 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 7 | 0.37 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 7 | 0.37 |
| (2,725) | 1:145:A:TYR:HD1 | 1:147:A:GLU:H | 10 | 0.37 |
| (2,725) | 1:145:A:TYR:HD2 | 1:147:A:GLU:H | 10 | 0.37 |
| (2,724) | 1:145:A:TYR:HD1 | 1:147:A:GLU:HG2 | 7 | 0.37 |
| (2,724) | 1:145:A:TYR:HD1 | 1:147:A:GLU:HG3 | 7 | 0.37 |
| (2,724) | 1:145:A:TYR:HD2 | 1:147:A:GLU:HG2 | 7 | 0.37 |
| (2,724) | 1:145:A:TYR:HD2 | 1:147:A:GLU:HG3 | 7 | 0.37 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 10 | 0.37 |
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 10 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 3 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 3 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 3 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 6 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 6 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 6 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 8 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 8 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 8 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG21 | 9 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG22 | 9 | 0.37 |
| (1,2098) | 1:153:A:ILE:HB | 1:153:A:ILE:HG23 | 9 | 0.37 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 9 | 0.37 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 9 | 0.37 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 9 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 1 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 1 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 1 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 2 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 2 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 2 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 4 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 4 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 4 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 5 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 5 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 5 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 6 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 6 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 6 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 7 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 7 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 7 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 9 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 9 | 0.37 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 9 | 0.37 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 2 | 0.37 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 2 | 0.37 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 2 | 0.37 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD21 | 7 | 0.37 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD22 | 7 | 0.37 |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H | 4 | 0.37 |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H | 4 | 0.37 |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H | 4 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 1 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 1 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 1 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 2 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 2 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 2 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 3 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 3 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 3 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 4 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 4 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 4 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 5 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 5 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 5 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 6 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 6 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 6 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 7 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 7 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 7 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 8 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 8 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 8 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 9 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 9 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 9 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 10 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 10 | 0.37 |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 10 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 3 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 3 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 3 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 6 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 6 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 6 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 7 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 7 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 7 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H | 10 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H | 10 | 0.37 |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H | 10 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 2 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 2 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 2 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 4 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 4 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 4 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 6 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 6 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 6 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 7 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 7 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 7 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 10 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 10 | 0.37 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 10 | 0.37 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 1 | 0.37 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 1 | 0.37 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG21 | 9 | 0.37 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG22 | 9 | 0.37 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG23 | 9 | 0.37 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG21 | 9 | 0.37 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG22 | 9 | 0.37 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG23 | 9 | 0.37 |
| (1,1050) | 1:76:A:TYR:HA | 1:76:A:TYR:HD1 | 10 | 0.37 |
| (1,1050) | 1:76:A:TYR:HA | 1:76:A:TYR:HD2 | 10 | 0.37 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 6 | 0.37 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 6 | 0.37 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 6 | 0.37 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 6 | 0.37 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 6 | 0.37 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 6 | 0.37 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD11 | 1 | 0.37 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD12 | 1 | 0.37 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD13 | 1 | 0.37 |
| (1,651) | 1:58:A:VAL:HG11 | 1:59:A:LYS:H | 2 | 0.37 |
| (1,651) | 1:58:A:VAL:HG12 | 1:59:A:LYS:H | 2 | 0.37 |
| (1,651) | 1:58:A:VAL:HG13 | 1:59:A:LYS:H | 2 | 0.37 |
| (1,651) | 1:58:A:VAL:HG21 | 1:59:A:LYS:H | 2 | 0.37 |
| (1,651) | 1:58:A:VAL:HG22 | 1:59:A:LYS:H | 2 | 0.37 |
| (1,651) | 1:58:A:VAL:HG23 | 1:59:A:LYS:H | 2 | 0.37 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 1 | 0.37 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 1 | 0.37 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 1 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 1 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 1 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 1 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 4 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 4 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 4 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 7 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 7 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 7 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 8 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 8 | 0.37 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 8 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 2 | 0.37 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 2 | 0.37 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 2 | 0.37 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 8 | 0.37 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 8 | 0.37 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 8 | 0.37 |
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 4 | 0.37 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 4 | 0.37 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 4 | 0.37 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 1 | 0.37 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 1 | 0.37 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 1 | 0.37 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 1 | 0.37 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 8 | 0.37 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 8 | 0.37 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 8 | 0.37 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 1 | 0.37 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 1 | 0.37 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 2 | 0.37 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 2 | 0.37 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 3 | 0.37 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 3 | 0.37 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 5 | 0.37 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 5 | 0.37 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 6 | 0.37 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 6 | 0.37 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 7 | 0.36 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 7 | 0.36 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 7 | 0.36 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 7 | 0.36 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 7 | 0.36 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 7 | 0.36 |
| (2,725) | 1:145:A:TYR:HD1 | 1:147:A:GLU:H | 8 | 0.36 |
| (2,725) | 1:145:A:TYR:HD2 | 1:147:A:GLU:H | 8 | 0.36 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 1 | 0.36 |
| (2,534) | 1:85:A:TYR:HE1 | 1:151:A:VAL:H | 1 | 0.36 |
| (2,534) | 1:85:A:TYR:HE2 | 1:151:A:VAL:H | 1 | 0.36 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD1 | 4 | 0.36 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD2 | 4 | 0.36 |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H | 8 | 0.36 |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H | 8 | 0.36 |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H | 8 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 3 | 0.36 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 3 | 0.36 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 3 | 0.36 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG21 | 10 | 0.36 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG22 | 10 | 0.36 |
| (1,2067) | 1:148:A:THR:HB | 1:148:A:THR:HG23 | 10 | 0.36 |
| (1,2054) | 1:145:A:TYR:HD1 | 1:146:A:ASN:H | 2 | 0.36 |
| (1,2054) | 1:145:A:TYR:HD2 | 1:146:A:ASN:H | 2 | 0.36 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 6 | 0.36 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 6 | 0.36 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 6 | 0.36 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 8 | 0.36 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 8 | 0.36 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 8 | 0.36 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 10 | 0.36 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 10 | 0.36 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 10 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 6 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 6 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 6 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 6 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 6 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 6 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 6 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 6 | 0.36 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 6 | 0.36 |
| (1,1707) | 1:115:A:LYS:HG2 | 1:116:A:GLU:H | 2 | 0.36 |
| (1,1707) | 1:115:A:LYS:HG3 | 1:116:A:GLU:H | 2 | 0.36 |
| (1,1707) | 1:115:A:LYS:HG2 | 1:116:A:GLU:H | 6 | 0.36 |
| (1,1707) | 1:115:A:LYS:HG3 | 1:116:A:GLU:H | 6 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 1 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 1 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 1 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 3 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 3 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 3 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 5 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 5 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 5 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 8 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 8 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 8 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG21 | 9 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG22 | 9 | 0.36 |
| (1,1447) | 1:90:A:THR:HB | 1:90:A:THR:HG23 | 9 | 0.36 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 3 | 0.36 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 3 | 0.36 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 3 | 0.36 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG21 | 5 | 0.36 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG22 | 5 | 0.36 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG23 | 5 | 0.36 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG21 | 5 | 0.36 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG22 | 5 | 0.36 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG23 | 5 | 0.36 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 7 | 0.36 |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H | 5 | 0.36 |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H | 5 | 0.36 |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H | 5 | 0.36 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 3 | 0.36 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 3 | 0.36 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 3 | 0.36 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB1 | 5 | 0.36 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB2 | 5 | 0.36 |
| (1,520) | 1:49:A:VAL:HB | 1:152:A:ALA:HB3 | 5 | 0.36 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 9 | 0.36 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 9 | 0.36 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 9 | 0.36 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 9 | 0.36 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 9 | 0.36 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 9 | 0.36 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 9 | 0.36 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 9 | 0.36 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 9 | 0.36 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD11 | 7 | 0.36 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD12 | 7 | 0.36 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD13 | 7 | 0.36 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 2 | 0.35 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 2 | 0.35 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD1 | 6 | 0.35 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD2 | 6 | 0.35 |
| (2,714) | 1:141:A:LYS:HD2 | 1:142:A:ILE:H | 6 | 0.35 |
| (2,714) | 1:141:A:LYS:HD3 | 1:142:A:ILE:H | 6 | 0.35 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG2 | 4 | 0.35 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG3 | 4 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,178) | 1:36:A:ALA:H | 1:37:A:GLY:H | 7 | 0.35 |
| (1,2327) | 1:171:A:LEU:HG | 1:171:A:LEU:H | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 9 | 0.35 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 9 | 0.35 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 2 | 0.35 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 2 | 0.35 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 2 | 0.35 |
| (1,2054) | 1:145:A:TYR:HD1 | 1:146:A:ASN:H | 1 | 0.35 |
| (1,2054) | 1:145:A:TYR:HD2 | 1:146:A:ASN:H | 1 | 0.35 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1 | 8 | 0.35 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2 | 8 | 0.35 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1 | 8 | 0.35 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2 | 8 | 0.35 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1 | 8 | 0.35 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2 | 8 | 0.35 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 6 | 0.35 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 6 | 0.35 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 6 | 0.35 |
| (1,1765) | 1:120:A:VAL:HB | 1:122:A:TYR:HE1 | 3 | 0.35 |
| (1,1765) | 1:120:A:VAL:HB | 1:122:A:TYR:HE2 | 3 | 0.35 |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H | 10 | 0.35 |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H | 10 | 0.35 |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H | 10 | 0.35 |
| (1,1707) | 1:115:A:LYS:HG2 | 1:116:A:GLU:H | 1 | 0.35 |
| (1,1707) | 1:115:A:LYS:HG3 | 1:116:A:GLU:H | 1 | 0.35 |
| (1,1707) | 1:115:A:LYS:HG2 | 1:116:A:GLU:H | 8 | 0.35 |
| (1,1707) | 1:115:A:LYS:HG3 | 1:116:A:GLU:H | 8 | 0.35 |
| (1,1556) | 1:103:A:SER:HA | 1:104:A:LEU:HB3 | 9 | 0.35 |
| (1,1556) | 1:103:A:SER:HA | 1:104:A:LEU:HB3 | 10 | 0.35 |
| (1,1475) | 1:95:A:PHE:HB2 | 1:96:A:SER:H | 10 | 0.35 |
| (1,1475) | 1:95:A:PHE:HB3 | 1:96:A:SER:H | 10 | 0.35 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 3 | 0.35 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 3 | 0.35 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 3 | 0.35 |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA | 2 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA | 2 | 0.35 |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA | 2 | 0.35 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 3 | 0.35 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 8 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD11 | 1:79:A:ILE:H | 5 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD12 | 1:79:A:ILE:H | 5 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD13 | 1:79:A:ILE:H | 5 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD21 | 1:79:A:ILE:H | 5 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD22 | 1:79:A:ILE:H | 5 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD23 | 1:79:A:ILE:H | 5 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD11 | 1:79:A:ILE:H | 6 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD12 | 1:79:A:ILE:H | 6 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD13 | 1:79:A:ILE:H | 6 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD21 | 1:79:A:ILE:H | 6 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD22 | 1:79:A:ILE:H | 6 | 0.35 |
| (1,1090) | 1:77:A:LEU:HD23 | 1:79:A:ILE:H | 6 | 0.35 |
| (1,965) | 1:72:A:PRO:HB2 | 1:73:A:TYR:HD1 | 10 | 0.35 |
| (1,965) | 1:72:A:PRO:HB2 | 1:73:A:TYR:HD2 | 10 | 0.35 |
| (1,922) | 1:70:A:LEU:HD11 | 1:70:A:LEU:H | 6 | 0.35 |
| (1,922) | 1:70:A:LEU:HD12 | 1:70:A:LEU:H | 6 | 0.35 |
| (1,922) | 1:70:A:LEU:HD13 | 1:70:A:LEU:H | 6 | 0.35 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 1 | 0.35 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 1 | 0.35 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 1 | 0.35 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 2 | 0.35 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 2 | 0.35 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 2 | 0.35 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG11 | 2 | 0.35 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG12 | 2 | 0.35 |
| (1,599) | 1:53:A:ASP:H | 1:55:A:VAL:HG13 | 2 | 0.35 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 5 | 0.35 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 5 | 0.35 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 5 | 0.35 |
| (1,356) | 1:42:A:ASP:HB2 | 1:160:A:TYR:HE1 | 6 | 0.35 |
| (1,356) | 1:42:A:ASP:HB2 | 1:160:A:TYR:HE2 | 6 | 0.35 |
| (1,356) | 1:42:A:ASP:HB3 | 1:160:A:TYR:HE1 | 6 | 0.35 |
| (1,356) | 1:42:A:ASP:HB3 | 1:160:A:TYR:HE2 | 6 | 0.35 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 2 | 0.35 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 5 | 0.35 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 5 | 0.35 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 5 | 0.35 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 5 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 5 | 0.35 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 5 | 0.35 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 5 | 0.35 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 5 | 0.35 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 5 | 0.35 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE1 | 3 | 0.34 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE2 | 3 | 0.34 |
| (2,129) | 1:28:A:HIS:H | 1:156:A:PHE:HE1 | 1 | 0.34 |
| (2,129) | 1:28:A:HIS:H | 1:156:A:PHE:HE2 | 1 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 2 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 2 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 2 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 2 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 2 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 2 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 2 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 2 | 0.34 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 2 | 0.34 |
| (1,2327) | 1:171:A:LEU:HG | 1:171:A:LEU:H | 7 | 0.34 |
| (1,2321) | 1:171:A:LEU:HD11 | 1:171:A:LEU:H | 6 | 0.34 |
| (1,2321) | 1:171:A:LEU:HD12 | 1:171:A:LEU:H | 6 | 0.34 |
| (1,2321) | 1:171:A:LEU:HD13 | 1:171:A:LEU:H | 6 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 1 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 10 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 10 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 10 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 10 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 10 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 10 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 10 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 10 | 0.34 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 10 | 0.34 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 8 | 0.34 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 8 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 8 | 0.34 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 8 | 0.34 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 8 | 0.34 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 8 | 0.34 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 5 | 0.34 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 5 | 0.34 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 5 | 0.34 |
| (1,2054) | 1:145:A:TYR:HD1 | 1:146:A:ASN:H | 4 | 0.34 |
| (1,2054) | 1:145:A:TYR:HD2 | 1:146:A:ASN:H | 4 | 0.34 |
| (1,2054) | 1:145:A:TYR:HD1 | 1:146:A:ASN:H | 9 | 0.34 |
| (1,2054) | 1:145:A:TYR:HD2 | 1:146:A:ASN:H | 9 | 0.34 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 3 | 0.34 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 3 | 0.34 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 3 | 0.34 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 2 | 0.34 |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 2 | 0.34 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 2 | 0.34 |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 2 | 0.34 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 2 | 0.34 |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 2 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 3 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 3 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 3 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 3 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 3 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 3 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 3 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 3 | 0.34 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 3 | 0.34 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG21 | 2 | 0.34 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG22 | 2 | 0.34 |
| (1,1844) | 1:132:A:SER:HB2 | 1:142:A:ILE:HG23 | 2 | 0.34 |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H | 4 | 0.34 |
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H | 4 | 0.34 |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H | 10 | 0.34 |
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H | 10 | 0.34 |
| (1,1556) | 1:103:A:SER:HA | 1:104:A:LEU:HB3 | 2 | 0.34 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 1 | 0.34 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 1 | 0.34 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 1 | 0.34 |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA | 3 | 0.34 |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA | 3 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA | 3 | 0.34 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 10 | 0.34 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD21 | 6 | 0.34 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD22 | 6 | 0.34 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD23 | 6 | 0.34 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 1 | 0.34 |
| (1,597) | 1:53:A:ASP:HB2 | 1:54:A:GLN:H | 6 | 0.34 |
| (1,597) | 1:53:A:ASP:HB3 | 1:54:A:GLN:H | 6 | 0.34 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 8 | 0.34 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 8 | 0.34 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 8 | 0.34 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 6 | 0.34 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 6 | 0.34 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 6 | 0.34 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 2 | 0.34 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 2 | 0.34 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 2 | 0.34 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 4 | 0.34 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 4 | 0.34 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 4 | 0.34 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE1 | 8 | 0.34 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE2 | 8 | 0.34 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 4 | 0.34 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 4 | 0.34 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 4 | 0.34 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 4 | 0.34 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 4 | 0.34 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 4 | 0.34 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE1 | 2 | 0.33 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE2 | 2 | 0.33 |
| (2,734) | 1:158:A:ALA:H | 1:159:A:PHE:HD1 | 10 | 0.33 |
| (2,734) | 1:158:A:ALA:H | 1:159:A:PHE:HD2 | 10 | 0.33 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 2 | 0.33 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 2 | 0.33 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 2 | 0.33 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 7 | 0.33 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 7 | 0.33 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 7 | 0.33 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 7 | 0.33 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 7 | 0.33 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 7 | 0.33 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 7 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 7 | 0.33 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 7 | 0.33 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 7 | 0.33 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 1 | 0.33 |
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 1 | 0.33 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 3 | 0.33 |
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 3 | 0.33 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 5 | 0.33 |
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 5 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HE1 | 2 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HE2 | 2 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HE1 | 2 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HE2 | 2 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HE1 | 2 | 0.33 |
| (1,2191) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HE2 | 2 | 0.33 |
| (1,2120) | 1:154:A:LEU:HG | 1:154:A:LEU:H | 2 | 0.33 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 8 | 0.33 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 8 | 0.33 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 8 | 0.33 |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H | 9 | 0.33 |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H | 9 | 0.33 |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H | 9 | 0.33 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 5 | 0.33 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 5 | 0.33 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 5 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 8 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 8 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 8 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 8 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 8 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 8 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 8 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 8 | 0.33 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 8 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1836) | 1:132:A:SER:HA | 1:145:A:TYR:HD1 | 4 | 0.33 |
| (1,1836) | 1:132:A:SER:HA | 1:145:A:TYR:HD2 | 4 | 0.33 |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H | 3 | 0.33 |
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H | 3 | 0.33 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD21 | 4 | 0.33 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD22 | 4 | 0.33 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD23 | 4 | 0.33 |
| (1,1557) | 1:103:A:SER:HA | 1:104:A:LEU:HB2 | 8 | 0.33 |
| (1,1556) | 1:103:A:SER:HA | 1:104:A:LEU:HB3 | 1 | 0.33 |
| (1,1556) | 1:103:A:SER:HA | 1:104:A:LEU:HB3 | 3 | 0.33 |
| (1,1338) | 1:85:A:TYR:HD1 | 1:86:A:GLU:H | 4 | 0.33 |
| (1,1338) | 1:85:A:TYR:HD2 | 1:86:A:GLU:H | 4 | 0.33 |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H | 7 | 0.33 |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H | 7 | 0.33 |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H | 7 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 8 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 8 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 8 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 8 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 8 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 8 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 8 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 8 | 0.33 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 8 | 0.33 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 6 | 0.33 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 6 | 0.33 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 6 | 0.33 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 7 | 0.33 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 7 | 0.33 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 7 | 0.33 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE1 | 7 | 0.33 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE2 | 7 | 0.33 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE1 | 3 | 0.33 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE2 | 3 | 0.33 |
| (1,238) | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB2 | 9 | 0.33 |
| (1,238) | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB3 | 9 | 0.33 |
| (1,238) | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB2 | 9 | 0.33 |
| (1,238) | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB3 | 9 | 0.33 |
| (1,238) | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB2 | 9 | 0.33 |
| (1,238) | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB3 | 9 | 0.33 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 3 | 0.33 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 3 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 3 | 0.33 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 9 | 0.33 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 9 | 0.33 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 9 | 0.33 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 6 | 0.32 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD11 | 7 | 0.32 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD12 | 7 | 0.32 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD13 | 7 | 0.32 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE1 | 5 | 0.32 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE2 | 5 | 0.32 |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 3 | 0.32 |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 3 | 0.32 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 3 | 0.32 |
| (2,601) | 1:115:A:LYS:HE2 | 1:116:A:GLU:H | 7 | 0.32 |
| (2,601) | 1:115:A:LYS:HE3 | 1:116:A:GLU:H | 7 | 0.32 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 6 | 0.32 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 6 | 0.32 |
| (2,397) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HA | 2 | 0.32 |
| (2,397) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HA | 2 | 0.32 |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H | 2 | 0.32 |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H | 2 | 0.32 |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H | 2 | 0.32 |
| (1,2446) | 1:179:A:VAL:HB | 1:179:A:VAL:H | 10 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 1 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 3 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 3 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 3 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 3 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 3 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 3 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 3 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 3 | 0.32 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 3 | 0.32 |
| (1,2327) | 1:171:A:LEU:HG | 1:171:A:LEU:H | 1 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 6 | 0.32 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 6 | 0.32 |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 6 | 0.32 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 6 | 0.32 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 6 | 0.32 |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 6 | 0.32 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 6 | 0.32 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 6 | 0.32 |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 6 | 0.32 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 7 | 0.32 |
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 7 | 0.32 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 1 | 0.32 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 1 | 0.32 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 1 | 0.32 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE1 | 8 | 0.32 |
| (1,2245) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HE2 | 8 | 0.32 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE1 | 8 | 0.32 |
| (1,2245) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HE2 | 8 | 0.32 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE1 | 8 | 0.32 |
| (1,2245) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HE2 | 8 | 0.32 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD21 | 4 | 0.32 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD22 | 4 | 0.32 |
| (1,2110) | 1:154:A:LEU:HA | 1:154:A:LEU:HD23 | 4 | 0.32 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 6 | 0.32 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 6 | 0.32 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 6 | 0.32 |
| (1,1970) | 1:138:A:GLU:HB2 | 1:138:A:GLU:H | 7 | 0.32 |
| (1,1970) | 1:138:A:GLU:HB3 | 1:138:A:GLU:H | 7 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 4 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 5 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 5 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 5 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 5 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 5 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 5 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 5 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 5 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 5 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 10 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 10 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 10 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 10 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 10 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 10 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 10 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 10 | 0.32 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 10 | 0.32 |
| (1,1557) | 1:103:A:SER:HA | 1:104:A:LEU:HB2 | 7 | 0.32 |
| (1,1485) | 1:95:A:PHE:HE1 | 1:117:A:ASP:HA | 2 | 0.32 |
| (1,1485) | 1:95:A:PHE:HE2 | 1:117:A:ASP:HA | 2 | 0.32 |
| (1,1400) | 1:87:A:THR:HG21 | 1:88:A:ASN:HA | 2 | 0.32 |
| (1,1400) | 1:87:A:THR:HG22 | 1:88:A:ASN:HA | 2 | 0.32 |
| (1,1400) | 1:87:A:THR:HG23 | 1:88:A:ASN:HA | 2 | 0.32 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 6 | 0.32 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 6 | 0.32 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 6 | 0.32 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 6 | 0.32 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 6 | 0.32 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 6 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB1 | 9 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB2 | 9 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB3 | 9 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB1 | 9 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB2 | 9 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB3 | 9 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB1 | 9 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB2 | 9 | 0.32 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB3 | 9 | 0.32 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 9 | 0.32 |
| (1,915) | 1:69:A:GLN:HG3 | 1:70:A:LEU:H | 10 | 0.32 |
| (1,909) | 1:69:A:GLN:HB2 | 1:70:A:LEU:H | 9 | 0.32 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 10 | 0.32 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 10 | 0.32 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 10 | 0.32 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 5 | 0.32 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 5 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 5 | 0.32 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 5 | 0.32 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 5 | 0.32 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 5 | 0.32 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 4 | 0.32 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 4 | 0.32 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 4 | 0.32 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 4 | 0.32 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 4 | 0.32 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 4 | 0.32 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 8 | 0.32 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 8 | 0.32 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 8 | 0.32 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 1 | 0.32 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 1 | 0.32 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 1 | 0.32 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 10 | 0.32 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 10 | 0.32 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 10 | 0.32 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 4 | 0.32 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 4 | 0.32 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 3 | 0.32 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 4 | 0.32 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 8 | 0.32 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 9 | 0.32 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 2 | 0.32 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 6 | 0.32 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 6 | 0.32 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 6 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 6 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 6 | 0.32 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 6 | 0.32 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 6 | 0.32 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 6 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 6 | 0.32 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 7 | 0.32 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 7 | 0.32 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 8 | 0.32 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 8 | 0.32 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 1 | 0.32 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 1 | 0.32 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 1 | 0.32 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 1 | 0.31 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 1 | 0.31 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 1 | 0.31 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 1 | 0.31 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 1 | 0.31 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 1 | 0.31 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 3 | 0.31 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 3 | 0.31 |
| (2,490) | 1:81:A:ILE:HD11 | 1:101:A:VAL:H | 5 | 0.31 |
| (2,490) | 1:81:A:ILE:HD12 | 1:101:A:VAL:H | 5 | 0.31 |
| (2,490) | 1:81:A:ILE:HD13 | 1:101:A:VAL:H | 5 | 0.31 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE1 | 6 | 0.31 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE2 | 6 | 0.31 |
| (2,355) | 1:64:A:LEU:H | 1:175:A:PHE:HE1 | 9 | 0.31 |
| (2,355) | 1:64:A:LEU:H | 1:175:A:PHE:HE2 | 9 | 0.31 |
| (2,295) | 1:52:A:LYS:HE2 | 1:54:A:GLN:HE22 | 3 | 0.31 |
| (2,295) | 1:52:A:LYS:HE3 | 1:54:A:GLN:HE22 | 3 | 0.31 |
| (1,2446) | 1:179:A:VAL:HB | 1:179:A:VAL:H | 2 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 6 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 10 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 10 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 10 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 10 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 10 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 10 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 10 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 10 | 0.31 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 10 | 0.31 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 8 | 0.31 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 8 | 0.31 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 8 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 1 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 2 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 7 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 9 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 9 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 9 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 9 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 9 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 9 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 9 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 9 | 0.31 |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 9 | 0.31 |
| (1,1845) | 1:132:A:SER:HB2 | 1:145:A:TYR:HD1 | 3 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1845) | 1:132:A:SER:HB2 | 1:145:A:TYR:HD2 | 3 | 0.31 |
| (1,1841) | 1:132:A:SER:HB3 | 1:145:A:TYR:HD1 | 2 | 0.31 |
| (1,1841) | 1:132:A:SER:HB3 | 1:145:A:TYR:HD2 | 2 | 0.31 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 10 | 0.31 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 10 | 0.31 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 10 | 0.31 |
| (1,1770) | 1:120:A:VAL:HG21 | 1:121:A:LEU:H | 4 | 0.31 |
| (1,1770) | 1:120:A:VAL:HG22 | 1:121:A:LEU:H | 4 | 0.31 |
| (1,1770) | 1:120:A:VAL:HG23 | 1:121:A:LEU:H | 4 | 0.31 |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H | 6 | 0.31 |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H | 6 | 0.31 |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H | 6 | 0.31 |
| (1,1557) | 1:103:A:SER:HA | 1:104:A:LEU:HB2 | 4 | 0.31 |
| (1,1556) | 1:103:A:SER:HA | 1:104:A:LEU:HB3 | 6 | 0.31 |
| (1,1483) | 1:95:A:PHE:HE1 | 1:116:A:GLU:HB3 | 5 | 0.31 |
| (1,1483) | 1:95:A:PHE:HE2 | 1:116:A:GLU:HB3 | 5 | 0.31 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 5 | 0.31 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 5 | 0.31 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 5 | 0.31 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 8 | 0.31 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 8 | 0.31 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 8 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG21 | 1 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG22 | 1 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG23 | 1 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG21 | 1 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG22 | 1 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG23 | 1 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG21 | 8 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG22 | 8 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG23 | 8 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG21 | 8 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG22 | 8 | 0.31 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG23 | 8 | 0.31 |
| (1,1032) | 1:74:A:PHE:HE1 | 1:168:A:PHE:HZ | 8 | 0.31 |
| (1,1032) | 1:74:A:PHE:HE2 | 1:168:A:PHE:HZ | 8 | 0.31 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 10 | 0.31 |
| (1,843) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD11 | 9 | 0.31 |
| (1,843) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD12 | 9 | 0.31 |
| (1,843) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD13 | 9 | 0.31 |
| (1,681) | 1:60:A:LEU:HD21 | 1:177:A:PHE:HD1 | 2 | 0.31 |
| (1,681) | 1:60:A:LEU:HD21 | 1:177:A:PHE:HD2 | 2 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,681) | 1:60:A:LEU:HD22 | 1:177:A:PHE:HD1 | 2 | 0.31 |
| (1,681) | 1:60:A:LEU:HD22 | 1:177:A:PHE:HD2 | 2 | 0.31 |
| (1,681) | 1:60:A:LEU:HD23 | 1:177:A:PHE:HD1 | 2 | 0.31 |
| (1,681) | 1:60:A:LEU:HD23 | 1:177:A:PHE:HD2 | 2 | 0.31 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 7 | 0.31 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 7 | 0.31 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 7 | 0.31 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 7 | 0.31 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 7 | 0.31 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 7 | 0.31 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 4 | 0.31 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 4 | 0.31 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 4 | 0.31 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 4 | 0.31 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 4 | 0.31 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 4 | 0.31 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 9 | 0.31 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 9 | 0.31 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 9 | 0.31 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 2 | 0.31 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 2 | 0.31 |
| (1,445) | 1:46:A:TYR:HE1 | 1:141:A:LYS:HE3 | 6 | 0.31 |
| (1,445) | 1:46:A:TYR:HE2 | 1:141:A:LYS:HE3 | 6 | 0.31 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE1 | 2 | 0.31 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE2 | 2 | 0.31 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 1 | 0.31 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 1 | 0.31 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 1 | 0.31 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 8 | 0.31 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 8 | 0.31 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 8 | 0.31 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE1 | 10 | 0.31 |
| (1,270) | 1:34:A:PRO:HD3 | 1:168:A:PHE:HE2 | 10 | 0.31 |
| (1,238) | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB2 | 6 | 0.31 |
| (1,238) | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB3 | 6 | 0.31 |
| (1,238) | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB2 | 6 | 0.31 |
| (1,238) | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB3 | 6 | 0.31 |
| (1,238) | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB2 | 6 | 0.31 |
| (1,238) | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB3 | 6 | 0.31 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 4 | 0.31 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 4 | 0.31 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 9 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 9 | 0.31 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 7 | 0.31 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 7 | 0.31 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 7 | 0.31 |
| (2,724) | 1:145:A:TYR:HD1 | 1:147:A:GLU:HG2 | 5 | 0.3 |
| (2,724) | 1:145:A:TYR:HD1 | 1:147:A:GLU:HG3 | 5 | 0.3 |
| (2,724) | 1:145:A:TYR:HD2 | 1:147:A:GLU:HG2 | 5 | 0.3 |
| (2,724) | 1:145:A:TYR:HD2 | 1:147:A:GLU:HG3 | 5 | 0.3 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE1 | 3 | 0.3 |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE2 | 3 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 4 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 5 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 8 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 9 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 9 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 9 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 9 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 9 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 9 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 9 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 9 | 0.3 |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 9 | 0.3 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 4 | 0.3 |
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 4 | 0.3 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 9 | 0.3 |
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 9 | 0.3 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 7 | 0.3 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 7 | 0.3 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 7 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 5 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 5 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 5 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 5 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 5 | 0.3 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 5 | 0.3 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 4 | 0.3 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 4 | 0.3 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 4 | 0.3 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 5 | 0.3 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 5 | 0.3 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 5 | 0.3 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 3 | 0.3 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 3 | 0.3 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 3 | 0.3 |
| (1,1845) | 1:132:A:SER:HB2 | 1:145:A:TYR:HD1 | 7 | 0.3 |
| (1,1845) | 1:132:A:SER:HB2 | 1:145:A:TYR:HD2 | 7 | 0.3 |
| (1,1841) | 1:132:A:SER:HB3 | 1:145:A:TYR:HD1 | 1 | 0.3 |
| (1,1841) | 1:132:A:SER:HB3 | 1:145:A:TYR:HD2 | 1 | 0.3 |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H | 1 | 0.3 |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H | 1 | 0.3 |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H | 1 | 0.3 |
| (1,1556) | 1:103:A:SER:HA | 1:104:A:LEU:HB3 | 5 | 0.3 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 5 | 0.3 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 5 | 0.3 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 5 | 0.3 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 7 | 0.3 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 7 | 0.3 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG21 | 4 | 0.3 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG22 | 4 | 0.3 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG23 | 4 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG21 | 4 | 0.3 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG22 | 4 | 0.3 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG23 | 4 | 0.3 |
| (1,1338) | 1:85:A:TYR:HD1 | 1:86:A:GLU:H | 10 | 0.3 |
| (1,1338) | 1:85:A:TYR:HD2 | 1:86:A:GLU:H | 10 | 0.3 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 7 | 0.3 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 7 | 0.3 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 7 | 0.3 |
| (1,1232) | 1:81:A:ILE:HG21 | 1:99:A:LYS:H | 3 | 0.3 |
| (1,1232) | 1:81:A:ILE:HG22 | 1:99:A:LYS:H | 3 | 0.3 |
| (1,1232) | 1:81:A:ILE:HG23 | 1:99:A:LYS:H | 3 | 0.3 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 4 | 0.3 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 5 | 0.3 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 2 | 0.3 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 2 | 0.3 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 2 | 0.3 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 5 | 0.3 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 5 | 0.3 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 5 | 0.3 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 3 | 0.3 |
| (1,242) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 3 | 0.3 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 3 | 0.3 |
| (1,242) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 3 | 0.3 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 3 | 0.3 |
| (1,242) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 3 | 0.3 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD11 | 4 | 0.3 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD12 | 4 | 0.3 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD13 | 4 | 0.3 |
| (1,123) | 1:27:A:SER:HB2 | 1:27:A:SER:H | 10 | 0.3 |
| (1,123) | 1:27:A:SER:HB3 | 1:27:A:SER:H | 10 | 0.3 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 5 | 0.3 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 5 | 0.3 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 5 | 0.3 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 4 | 0.29 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 4 | 0.29 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 4 | 0.29 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 10 | 0.29 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 10 | 0.29 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 10 | 0.29 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 4 | 0.29 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 4 | 0.29 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 4 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 10 | 0.29 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 10 | 0.29 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 10 | 0.29 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE1 | 10 | 0.29 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE2 | 10 | 0.29 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD1 | 3 | 0.29 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD2 | 3 | 0.29 |
| (1,2327) | 1:171:A:LEU:HG | 1:171:A:LEU:H | 6 | 0.29 |
| (1,2262) | 1:164:A:GLU:HA | 1:164:A:GLU:HG2 | 4 | 0.29 |
| (1,2262) | 1:164:A:GLU:HA | 1:164:A:GLU:HG3 | 4 | 0.29 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 1 | 0.29 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 1 | 0.29 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 1 | 0.29 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 1 | 0.29 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 1 | 0.29 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 1 | 0.29 |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H | 5 | 0.29 |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H | 5 | 0.29 |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H | 5 | 0.29 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 6 | 0.29 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 6 | 0.29 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 6 | 0.29 |
| (1,1485) | 1:95:A:PHE:HE1 | 1:117:A:ASP:HA | 9 | 0.29 |
| (1,1485) | 1:95:A:PHE:HE2 | 1:117:A:ASP:HA | 9 | 0.29 |
| (1,1485) | 1:95:A:PHE:HE1 | 1:117:A:ASP:HA | 10 | 0.29 |
| (1,1485) | 1:95:A:PHE:HE2 | 1:117:A:ASP:HA | 10 | 0.29 |
| (1,1483) | 1:95:A:PHE:HE1 | 1:116:A:GLU:HB3 | 1 | 0.29 |
| (1,1483) | 1:95:A:PHE:HE2 | 1:116:A:GLU:HB3 | 1 | 0.29 |
| (1,1483) | 1:95:A:PHE:HE1 | 1:116:A:GLU:HB3 | 4 | 0.29 |
| (1,1483) | 1:95:A:PHE:HE2 | 1:116:A:GLU:HB3 | 4 | 0.29 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 5 | 0.29 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 5 | 0.29 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 5 | 0.29 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 8 | 0.29 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 8 | 0.29 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 2 | 0.29 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 2 | 0.29 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 2 | 0.29 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 1 | 0.29 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 6 | 0.29 |
| (1,1071) | 1:76:A:TYR:HE1 | 1:160:A:TYR:HA | 7 | 0.29 |
| (1,1071) | 1:76:A:TYR:HE2 | 1:160:A:TYR:HA | 7 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1020) | 1:74:A:PHE:HD1 | 1:162:A:ALA:HA | 8 | 0.29 |
| (1,1020) | 1:74:A:PHE:HD2 | 1:162:A:ALA:HA | 8 | 0.29 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 5 | 0.29 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 5 | 0.29 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 5 | 0.29 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 7 | 0.29 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 7 | 0.29 |
| (1,852) | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 7 | 0.29 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 9 | 0.29 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 9 | 0.29 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 9 | 0.29 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 1 | 0.29 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 1 | 0.29 |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 1 | 0.29 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 5 | 0.29 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 5 | 0.29 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 7 | 0.29 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 7 | 0.29 |
| (1,456) | 1:47:A:ALA:HB1 | 1:156:A:PHE:HZ | 1 | 0.29 |
| (1,456) | 1:47:A:ALA:HB2 | 1:156:A:PHE:HZ | 1 | 0.29 |
| (1,456) | 1:47:A:ALA:HB3 | 1:156:A:PHE:HZ | 1 | 0.29 |
| (1,455) | 1:47:A:ALA:HB1 | 1:48:A:ILE:H | 1 | 0.29 |
| (1,455) | 1:47:A:ALA:HB2 | 1:48:A:ILE:H | 1 | 0.29 |
| (1,455) | 1:47:A:ALA:HB3 | 1:48:A:ILE:H | 1 | 0.29 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB1 | 3 | 0.29 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB2 | 3 | 0.29 |
| (1,353) | 1:42:A:ASP:HB2 | 1:158:A:ALA:HB3 | 3 | 0.29 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB1 | 3 | 0.29 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB2 | 3 | 0.29 |
| (1,353) | 1:42:A:ASP:HB3 | 1:158:A:ALA:HB3 | 3 | 0.29 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 2 | 0.29 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 2 | 0.29 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 2 | 0.29 |
| (1,166) | 1:29:A:LEU:HD11 | 1:175:A:PHE:H | 10 | 0.29 |
| (1,166) | 1:29:A:LEU:HD12 | 1:175:A:PHE:H | 10 | 0.29 |
| (1,166) | 1:29:A:LEU:HD13 | 1:175:A:PHE:H | 10 | 0.29 |
| (1,11) | 1:20:A:SER:HB2 | 1:21:A:GLU:H | 1 | 0.29 |
| (1,11) | 1:20:A:SER:HB3 | 1:21:A:GLU:H | 1 | 0.29 |
| (1,3) | 1:16:A:ALA:HB1 | 1:16:A:ALA:H | 8 | 0.29 |
| (1,3) | 1:16:A:ALA:HB2 | 1:16:A:ALA:H | 8 | 0.29 |
| (1,3) | 1:16:A:ALA:HB3 | 1:16:A:ALA:H | 8 | 0.29 |
| (2,714) | 1:141:A:LYS:HD2 | 1:142:A:ILE:H | 1 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,714) | 1:141:A:LYS:HD3 | 1:142:A:ILE:H | 1 | 0.28 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 6 | 0.28 |
| (2,625) | 1:121:A:LEU:H | 1:122:A:TYR:HD1 | 7 | 0.28 |
| (2,625) | 1:121:A:LEU:H | 1:122:A:TYR:HD2 | 7 | 0.28 |
| (2,567) | 1:90:A:THR:HG21 | 1:92:A:LEU:H | 9 | 0.28 |
| (2,567) | 1:90:A:THR:HG22 | 1:92:A:LEU:H | 9 | 0.28 |
| (2,567) | 1:90:A:THR:HG23 | 1:92:A:LEU:H | 9 | 0.28 |
| (2,547) | 1:87:A:THR:HG21 | 1:91:A:ALA:H | 2 | 0.28 |
| (2,547) | 1:87:A:THR:HG22 | 1:91:A:ALA:H | 2 | 0.28 |
| (2,547) | 1:87:A:THR:HG23 | 1:91:A:ALA:H | 2 | 0.28 |
| (2,522) | 1:85:A:TYR:HD1 | 1:134:A:TRP:HA | 3 | 0.28 |
| (2,522) | 1:85:A:TYR:HD2 | 1:134:A:TRP:HA | 3 | 0.28 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 4 | 0.28 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 4 | 0.28 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 4 | 0.28 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 4 | 0.28 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG21 | 2 | 0.28 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG22 | 2 | 0.28 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG23 | 2 | 0.28 |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H | 5 | 0.28 |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H | 5 | 0.28 |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H | 5 | 0.28 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD11 | 1 | 0.28 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD12 | 1 | 0.28 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD13 | 1 | 0.28 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 4 | 0.28 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 4 | 0.28 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 4 | 0.28 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 6 | 0.28 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 9 | 0.28 |
| (1,2053) | 1:145:A:TYR:HD1 | 1:145:A:TYR:H | 6 | 0.28 |
| (1,2053) | 1:145:A:TYR:HD2 | 1:145:A:TYR:H | 6 | 0.28 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 2 | 0.28 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 2 | 0.28 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 2 | 0.28 |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H | 3 | 0.28 |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H | 3 | 0.28 |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H | 3 | 0.28 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 4 | 0.28 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 4 | 0.28 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 4 | 0.28 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 7 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 7 | 0.28 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 7 | 0.28 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 9 | 0.28 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 9 | 0.28 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 9 | 0.28 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 1 | 0.28 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 1 | 0.28 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD21 | 4 | 0.28 |
| (1,1954) | 1:136:A:PRO:HG2 | 1:155:A:ASN:HD22 | 4 | 0.28 |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB | 8 | 0.28 |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB | 8 | 0.28 |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB | 8 | 0.28 |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H | 3 | 0.28 |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H | 3 | 0.28 |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H | 3 | 0.28 |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H | 1 | 0.28 |
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H | 1 | 0.28 |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H | 8 | 0.28 |
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H | 8 | 0.28 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD21 | 10 | 0.28 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD22 | 10 | 0.28 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD23 | 10 | 0.28 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 9 | 0.28 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 9 | 0.28 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 9 | 0.28 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 2 | 0.28 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 1 | 0.28 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 9 | 0.28 |
| (1,999) | 1:74:A:PHE:HA | 1:74:A:PHE:HD1 | 8 | 0.28 |
| (1,999) | 1:74:A:PHE:HA | 1:74:A:PHE:HD2 | 8 | 0.28 |
| (1,908) | 1:69:A:GLN:HB3 | 1:70:A:LEU:H | 10 | 0.28 |
| (1,873) | 1:67:A:ALA:HB1 | 1:68:A:GLU:H | 4 | 0.28 |
| (1,873) | 1:67:A:ALA:HB2 | 1:68:A:GLU:H | 4 | 0.28 |
| (1,873) | 1:67:A:ALA:HB3 | 1:68:A:GLU:H | 4 | 0.28 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD21 | 1 | 0.28 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD22 | 1 | 0.28 |
| (1,844) | 1:66:A:ASN:HD21 | 1:70:A:LEU:HD23 | 1 | 0.28 |
| (1,755) | 1:63:A:THR:HG21 | 1:108:A:SER:HA | 10 | 0.28 |
| (1,755) | 1:63:A:THR:HG22 | 1:108:A:SER:HA | 10 | 0.28 |
| (1,755) | 1:63:A:THR:HG23 | 1:108:A:SER:HA | 10 | 0.28 |
| (1,727) | 1:62:A:VAL:HG11 | 1:177:A:PHE:HE1 | 5 | 0.28 |
| (1,727) | 1:62:A:VAL:HG11 | 1:177:A:PHE:HE2 | 5 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,727) | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE1 | 5 | 0.28 |
| (1,727) | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE2 | 5 | 0.28 |
| (1,727) | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE1 | 5 | 0.28 |
| (1,727) | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE2 | 5 | 0.28 |
| (1,724) | 1:62:A:VAL:HG11 | 1:63:A:THR:H | 5 | 0.28 |
| (1,724) | 1:62:A:VAL:HG12 | 1:63:A:THR:H | 5 | 0.28 |
| (1,724) | 1:62:A:VAL:HG13 | 1:63:A:THR:H | 5 | 0.28 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 3 | 0.28 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 3 | 0.28 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 3 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 3 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 3 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 3 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 4 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 4 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 4 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 8 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 8 | 0.28 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 8 | 0.28 |
| (1,597) | 1:53:A:ASP:HB2 | 1:54:A:GLN:H | 5 | 0.28 |
| (1,597) | 1:53:A:ASP:HB3 | 1:54:A:GLN:H | 5 | 0.28 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 5 | 0.28 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 5 | 0.28 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 5 | 0.28 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG21 | 3 | 0.28 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG22 | 3 | 0.28 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG23 | 3 | 0.28 |
| (1,362) | 1:42:A:ASP:H | 1:160:A:TYR:HE1 | 1 | 0.28 |
| (1,362) | 1:42:A:ASP:H | 1:160:A:TYR:HE2 | 1 | 0.28 |
| (1,286) | 1:36:A:ALA:HA | 1:37:A:GLY:H | 10 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 3 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 3 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 3 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 4 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 4 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 4 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 5 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 5 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 5 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 6 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 6 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 6 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 7 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 7 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 7 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 8 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 8 | 0.28 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 8 | 0.28 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD11 | 3 | 0.28 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD12 | 3 | 0.28 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD13 | 3 | 0.28 |
| (1,171) | 1:29:A:LEU:HD21 | 1:175:A:PHE:H | 2 | 0.28 |
| (1,171) | 1:29:A:LEU:HD22 | 1:175:A:PHE:H | 2 | 0.28 |
| (1,171) | 1:29:A:LEU:HD23 | 1:175:A:PHE:H | 2 | 0.28 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 5 | 0.28 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 5 | 0.28 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 5 | 0.28 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 5 | 0.28 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 5 | 0.28 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 5 | 0.28 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 8 | 0.28 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 8 | 0.28 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 8 | 0.28 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 8 | 0.28 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 8 | 0.28 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 8 | 0.28 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 3 | 0.27 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 9 | 0.27 |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 9 | 0.27 |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 9 | 0.27 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 9 | 0.27 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 6 | 0.27 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 6 | 0.27 |
| (2,523) | 1:85:A:TYR:HD1 | 1:134:A:TRP:H | 9 | 0.27 |
| (2,523) | 1:85:A:TYR:HD2 | 1:134:A:TRP:H | 9 | 0.27 |
| (2,468) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HE1 | 6 | 0.27 |
| (2,468) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HE2 | 6 | 0.27 |
| (2,468) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HE1 | 6 | 0.27 |
| (2,468) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HE2 | 6 | 0.27 |
| (2,468) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HE1 | 6 | 0.27 |
| (2,468) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HE2 | 6 | 0.27 |
| (2,397) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HA | 9 | 0.27 |
| (2,397) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HA | 9 | 0.27 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD1 | 5 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD2 | 5 | 0.27 |
| (2,178) | 1:36:A:ALA:H | 1:37:A:GLY:H | 10 | 0.27 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE1 | 7 | 0.27 |
| (2,125) | 1:28:A:HIS:HE1 | 1:46:A:TYR:HE2 | 7 | 0.27 |
| (1,2262) | 1:164:A:GLU:HA | 1:164:A:GLU:HG2 | 2 | 0.27 |
| (1,2262) | 1:164:A:GLU:HA | 1:164:A:GLU:HG3 | 2 | 0.27 |
| (1,2262) | 1:164:A:GLU:HA | 1:164:A:GLU:HG2 | 5 | 0.27 |
| (1,2262) | 1:164:A:GLU:HA | 1:164:A:GLU:HG3 | 5 | 0.27 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 9 | 0.27 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 9 | 0.27 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 9 | 0.27 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 1 | 0.27 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 4 | 0.27 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 8 | 0.27 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 9 | 0.27 |
| (1,2043) | 1:145:A:TYR:HA | 1:145:A:TYR:HD1 | 4 | 0.27 |
| (1,2043) | 1:145:A:TYR:HA | 1:145:A:TYR:HD2 | 4 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 1 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 1 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 1 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 1 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 1 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 1 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 1 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 1 | 0.27 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 1 | 0.27 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD11 | 2 | 0.27 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD12 | 2 | 0.27 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD13 | 2 | 0.27 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 8 | 0.27 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 8 | 0.27 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 8 | 0.27 |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H | 7 | 0.27 |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H | 7 | 0.27 |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H | 7 | 0.27 |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB | 2 | 0.27 |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB | 2 | 0.27 |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB | 2 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H | 1 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H | 1 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H | 1 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H | 2 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H | 2 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H | 2 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H | 9 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H | 9 | 0.27 |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H | 9 | 0.27 |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA | 2 | 0.27 |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA | 2 | 0.27 |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA | 2 | 0.27 |
| (1,1474) | 1:95:A:PHE:HB2 | 1:95:A:PHE:H | 6 | 0.27 |
| (1,1474) | 1:95:A:PHE:HB3 | 1:95:A:PHE:H | 6 | 0.27 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 3 | 0.27 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 3 | 0.27 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 3 | 0.27 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG21 | 7 | 0.27 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG22 | 7 | 0.27 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG23 | 7 | 0.27 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG21 | 7 | 0.27 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG22 | 7 | 0.27 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG23 | 7 | 0.27 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD21 | 1 | 0.27 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD22 | 1 | 0.27 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD23 | 1 | 0.27 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD21 | 10 | 0.27 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD22 | 10 | 0.27 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD23 | 10 | 0.27 |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H | 3 | 0.27 |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H | 3 | 0.27 |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H | 3 | 0.27 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG21 | 10 | 0.27 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG22 | 10 | 0.27 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG23 | 10 | 0.27 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG21 | 10 | 0.27 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG22 | 10 | 0.27 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG23 | 10 | 0.27 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 3 | 0.27 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 8 | 0.27 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 10 | 0.27 |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H | 2 | 0.27 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 8 | 0.27 |
| (1,873) | 1:67:A:ALA:HB1 | 1:68:A:GLU:H | 7 | 0.27 |
| (1,873) | 1:67:A:ALA:HB2 | 1:68:A:GLU:H | 7 | 0.27 |
| (1,873) | 1:67:A:ALA:HB3 | 1:68:A:GLU:H | 7 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 4 | 0.27 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 4 | 0.27 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 4 | 0.27 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 4 | 0.27 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 4 | 0.27 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 4 | 0.27 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 4 | 0.27 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 4 | 0.27 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 4 | 0.27 |
| (1,755) | 1:63:A:THR:HG21 | 1:108:A:SER:HA | 9 | 0.27 |
| (1,755) | 1:63:A:THR:HG22 | 1:108:A:SER:HA | 9 | 0.27 |
| (1,755) | 1:63:A:THR:HG23 | 1:108:A:SER:HA | 9 | 0.27 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 7 | 0.27 |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 7 | 0.27 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 7 | 0.27 |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 7 | 0.27 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 7 | 0.27 |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 7 | 0.27 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 9 | 0.27 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 9 | 0.27 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 9 | 0.27 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 3 | 0.27 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 3 | 0.27 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 3 | 0.27 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 9 | 0.27 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 9 | 0.27 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 9 | 0.27 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 2 | 0.27 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 4 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 1 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 1 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 1 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 9 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 9 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 9 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG21 | 10 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG22 | 10 | 0.27 |
| (1,257) | 1:33:A:THR:HB | 1:33:A:THR:HG23 | 10 | 0.27 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 10 | 0.27 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 10 | 0.27 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 10 | 0.27 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 10 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 10 | 0.27 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 10 | 0.27 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE1 | 1 | 0.26 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE2 | 1 | 0.26 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE1 | 5 | 0.26 |
| (2,735) | 1:158:A:ALA:H | 1:160:A:TYR:HE2 | 5 | 0.26 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD1 | 3 | 0.26 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD2 | 3 | 0.26 |
| (2,709) | 1:133:A:ILE:HD11 | 1:147:A:GLU:H | 6 | 0.26 |
| (2,709) | 1:133:A:ILE:HD12 | 1:147:A:GLU:H | 6 | 0.26 |
| (2,709) | 1:133:A:ILE:HD13 | 1:147:A:GLU:H | 6 | 0.26 |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H | 2 | 0.26 |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H | 2 | 0.26 |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H | 1 | 0.26 |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H | 1 | 0.26 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 1 | 0.26 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 1 | 0.26 |
| (2,522) | 1:85:A:TYR:HD1 | 1:134:A:TRP:HA | 10 | 0.26 |
| (2,522) | 1:85:A:TYR:HD2 | 1:134:A:TRP:HA | 10 | 0.26 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG21 | 5 | 0.26 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG22 | 5 | 0.26 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG23 | 5 | 0.26 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG21 | 9 | 0.26 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG22 | 9 | 0.26 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG23 | 9 | 0.26 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 1 | 0.26 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 1 | 0.26 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 1 | 0.26 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 2 | 0.26 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 2 | 0.26 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 2 | 0.26 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 2 | 0.26 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 2 | 0.26 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 2 | 0.26 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 2 | 0.26 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 5 | 0.26 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 6 | 0.26 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 7 | 0.26 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD11 | 1 | 0.26 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD12 | 1 | 0.26 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD13 | 1 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 2 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 2 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 2 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 3 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 3 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 3 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 10 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 10 | 0.26 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 10 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG2 | 1:125:A:LYS:HE2 | 5 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG2 | 1:125:A:LYS:HE3 | 5 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG3 | 1:125:A:LYS:HE2 | 5 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG3 | 1:125:A:LYS:HE3 | 5 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG2 | 1:125:A:LYS:HE2 | 6 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG2 | 1:125:A:LYS:HE3 | 6 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG3 | 1:125:A:LYS:HE2 | 6 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG3 | 1:125:A:LYS:HE3 | 6 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG2 | 1:125:A:LYS:HE2 | 8 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG2 | 1:125:A:LYS:HE3 | 8 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG3 | 1:125:A:LYS:HE2 | 8 | 0.26 |
| (1,1789) | 1:125:A:LYS:HG3 | 1:125:A:LYS:HE3 | 8 | 0.26 |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H | 2 | 0.26 |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H | 2 | 0.26 |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H | 2 | 0.26 |
| (1,1723) | 1:116:A:GLU:HG2 | 1:116:A:GLU:H | 10 | 0.26 |
| (1,1723) | 1:116:A:GLU:HG3 | 1:116:A:GLU:H | 10 | 0.26 |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA | 10 | 0.26 |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA | 10 | 0.26 |
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA | 10 | 0.26 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD11 | 5 | 0.26 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD12 | 5 | 0.26 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD13 | 5 | 0.26 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 1 | 0.26 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 1 | 0.26 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 1 | 0.26 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 10 | 0.26 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 10 | 0.26 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 10 | 0.26 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 10 | 0.26 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 10 | 0.26 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 10 | 0.26 |
| (1,1338) | 1:85:A:TYR:HD1 | 1:86:A:GLU:H | 3 | 0.26 |
| (1,1338) | 1:85:A:TYR:HD2 | 1:86:A:GLU:H | 3 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 10 | 0.26 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 4 | 0.26 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 7 | 0.26 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 10 | 0.26 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 7 | 0.26 |
| (1,873) | 1:67:A:ALA:HB1 | 1:68:A:GLU:H | 1 | 0.26 |
| (1,873) | 1:67:A:ALA:HB2 | 1:68:A:GLU:H | 1 | 0.26 |
| (1,873) | 1:67:A:ALA:HB3 | 1:68:A:GLU:H | 1 | 0.26 |
| (1,724) | 1:62:A:VAL:HG11 | 1:63:A:THR:H | 3 | 0.26 |
| (1,724) | 1:62:A:VAL:HG12 | 1:63:A:THR:H | 3 | 0.26 |
| (1,724) | 1:62:A:VAL:HG13 | 1:63:A:THR:H | 3 | 0.26 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 4 | 0.26 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 4 | 0.26 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 4 | 0.26 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 9 | 0.26 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 9 | 0.26 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 9 | 0.26 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 6 | 0.26 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG11 | 10 | 0.26 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG12 | 10 | 0.26 |
| (1,610) | 1:55:A:VAL:HA | 1:55:A:VAL:HG13 | 10 | 0.26 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 4 | 0.26 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 4 | 0.26 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 4 | 0.26 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG21 | 1 | 0.26 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG22 | 1 | 0.26 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG23 | 1 | 0.26 |
| (1,299) | 1:39:A:GLN:HA | 1:39:A:GLN:H | 10 | 0.26 |
| (1,292) | 1:37:A:GLY:HA2 | 1:37:A:GLY:H | 10 | 0.26 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 8 | 0.26 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 8 | 0.26 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 8 | 0.26 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 8 | 0.26 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 8 | 0.26 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 8 | 0.26 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 8 | 0.26 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 8 | 0.26 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 8 | 0.26 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 1 | 0.26 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 4 | 0.26 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 5 | 0.25 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 7 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 8 | 0.25 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 8 | 0.25 |
| (2,673) | 1:127:A:GLY:H | 1:128:A:TYR:HD1 | 6 | 0.25 |
| (2,673) | 1:127:A:GLY:H | 1:128:A:TYR:HD2 | 6 | 0.25 |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA | 7 | 0.25 |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA | 7 | 0.25 |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA | 7 | 0.25 |
| (2,552) | 1:87:A:THR:H | 1:92:A:LEU:HB2 | 2 | 0.25 |
| (2,468) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HE1 | 5 | 0.25 |
| (2,468) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HE2 | 5 | 0.25 |
| (2,468) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HE1 | 5 | 0.25 |
| (2,468) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HE2 | 5 | 0.25 |
| (2,468) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HE1 | 5 | 0.25 |
| (2,468) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HE2 | 5 | 0.25 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD1 | 10 | 0.25 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD2 | 10 | 0.25 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 7 | 0.25 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 7 | 0.25 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 7 | 0.25 |
| (1,2425) | 1:177:A:PHE:HD1 | 1:177:A:PHE:H | 4 | 0.25 |
| (1,2425) | 1:177:A:PHE:HD2 | 1:177:A:PHE:H | 4 | 0.25 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 3 | 0.25 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 3 | 0.25 |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 3 | 0.25 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 5 | 0.25 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 5 | 0.25 |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 5 | 0.25 |
| (1,2327) | 1:171:A:LEU:HG | 1:171:A:LEU:H | 8 | 0.25 |
| (1,2327) | 1:171:A:LEU:HG | 1:171:A:LEU:H | 10 | 0.25 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 3 | 0.25 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 7 | 0.25 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 1 | 0.25 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 4 | 0.25 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 5 | 0.25 |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H | 9 | 0.25 |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H | 9 | 0.25 |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H | 9 | 0.25 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD11 | 10 | 0.25 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD12 | 10 | 0.25 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD13 | 10 | 0.25 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1 | 7 | 0.25 |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2 | 7 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1 | 7 | 0.25 |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2 | 7 | 0.25 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1 | 7 | 0.25 |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2 | 7 | 0.25 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG21 | 9 | 0.25 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG22 | 9 | 0.25 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG23 | 9 | 0.25 |
| (1,1793) | 1:128:A:TYR:HA | 1:128:A:TYR:HB3 | 3 | 0.25 |
| (1,1770) | 1:120:A:VAL:HG21 | 1:121:A:LEU:H | 10 | 0.25 |
| (1,1770) | 1:120:A:VAL:HG22 | 1:121:A:LEU:H | 10 | 0.25 |
| (1,1770) | 1:120:A:VAL:HG23 | 1:121:A:LEU:H | 10 | 0.25 |
| (1,1768) | 1:120:A:VAL:HG11 | 1:122:A:TYR:HE1 | 4 | 0.25 |
| (1,1768) | 1:120:A:VAL:HG11 | 1:122:A:TYR:HE2 | 4 | 0.25 |
| (1,1768) | 1:120:A:VAL:HG12 | 1:122:A:TYR:HE1 | 4 | 0.25 |
| (1,1768) | 1:120:A:VAL:HG12 | 1:122:A:TYR:HE2 | 4 | 0.25 |
| (1,1768) | 1:120:A:VAL:HG13 | 1:122:A:TYR:HE1 | 4 | 0.25 |
| (1,1768) | 1:120:A:VAL:HG13 | 1:122:A:TYR:HE2 | 4 | 0.25 |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H | 5 | 0.25 |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H | 5 | 0.25 |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H | 5 | 0.25 |
| (1,1474) | 1:95:A:PHE:HB2 | 1:95:A:PHE:H | 3 | 0.25 |
| (1,1474) | 1:95:A:PHE:HB3 | 1:95:A:PHE:H | 3 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 4 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 4 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 4 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 5 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 5 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 5 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 6 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 6 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 6 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 8 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 8 | 0.25 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 8 | 0.25 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 2 | 0.25 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 2 | 0.25 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD21 | 5 | 0.25 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD22 | 5 | 0.25 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD23 | 5 | 0.25 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 7 | 0.25 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 7 | 0.25 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 7 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE1 | 2 | 0.25 |
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE2 | 2 | 0.25 |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE1 | 2 | 0.25 |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE2 | 2 | 0.25 |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE1 | 2 | 0.25 |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE2 | 2 | 0.25 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG21 | 4 | 0.25 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG22 | 4 | 0.25 |
| (1,1189) | 1:80:A:GLN:HG2 | 1:98:A:THR:HG23 | 4 | 0.25 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG21 | 4 | 0.25 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG22 | 4 | 0.25 |
| (1,1189) | 1:80:A:GLN:HG3 | 1:98:A:THR:HG23 | 4 | 0.25 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 6 | 0.25 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 9 | 0.25 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 3 | 0.25 |
| (1,1032) | 1:74:A:PHE:HE1 | 1:168:A:PHE:HZ | 6 | 0.25 |
| (1,1032) | 1:74:A:PHE:HE2 | 1:168:A:PHE:HZ | 6 | 0.25 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 2 | 0.25 |
| (1,924) | 1:70:A:LEU:HD11 | 1:74:A:PHE:HD1 | 1 | 0.25 |
| (1,924) | 1:70:A:LEU:HD11 | 1:74:A:PHE:HD2 | 1 | 0.25 |
| (1,924) | 1:70:A:LEU:HD12 | 1:74:A:PHE:HD1 | 1 | 0.25 |
| (1,924) | 1:70:A:LEU:HD12 | 1:74:A:PHE:HD2 | 1 | 0.25 |
| (1,924) | 1:70:A:LEU:HD13 | 1:74:A:PHE:HD1 | 1 | 0.25 |
| (1,924) | 1:70:A:LEU:HD13 | 1:74:A:PHE:HD2 | 1 | 0.25 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 3 | 0.25 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 3 | 0.25 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 3 | 0.25 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 3 | 0.25 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 3 | 0.25 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 3 | 0.25 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 3 | 0.25 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 3 | 0.25 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 3 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 1 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 1 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 1 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 5 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 5 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 5 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 7 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 7 | 0.25 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 7 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 3 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 3 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 3 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 6 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 6 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 6 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 9 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 9 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 9 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 10 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 10 | 0.25 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 10 | 0.25 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 1 | 0.25 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 1 | 0.25 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 1 | 0.25 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 4 | 0.25 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 7 | 0.25 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 8 | 0.25 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 3 | 0.25 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 3 | 0.25 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 3 | 0.25 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 3 | 0.25 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 3 | 0.25 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 3 | 0.25 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 3 | 0.25 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 3 | 0.25 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 3 | 0.25 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD11 | 10 | 0.25 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD12 | 10 | 0.25 |
| (1,212) | 1:32:A:ILE:HB | 1:32:A:ILE:HD13 | 10 | 0.25 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 3 | 0.25 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 3 | 0.25 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 3 | 0.25 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 3 | 0.25 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 3 | 0.25 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 3 | 0.25 |
| (1,126) | 1:27:A:SER:HB2 | 1:177:A:PHE:HE1 | 7 | 0.25 |
| (1,126) | 1:27:A:SER:HB2 | 1:177:A:PHE:HE2 | 7 | 0.25 |
| (1,126) | 1:27:A:SER:HB3 | 1:177:A:PHE:HE1 | 7 | 0.25 |
| (1,126) | 1:27:A:SER:HB3 | 1:177:A:PHE:HE2 | 7 | 0.25 |
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG21 | 7 | 0.25 |
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG22 | 7 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,86) | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG23 | 7 | 0.25 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG21 | 7 | 0.25 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG22 | 7 | 0.25 |
| (1,86) | 1:25:A:VAL:HG22 | 1:49:A:VAL:HG23 | 7 | 0.25 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG21 | 7 | 0.25 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG22 | 7 | 0.25 |
| (1,86) | 1:25:A:VAL:HG23 | 1:49:A:VAL:HG23 | 7 | 0.25 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 9 | 0.24 |
| (2,689) | 1:131:A:THR:HA | 1:145:A:TYR:HD1 | 3 | 0.24 |
| (2,689) | 1:131:A:THR:HA | 1:145:A:TYR:HD2 | 3 | 0.24 |
| (2,673) | 1:127:A:GLY:H | 1:128:A:TYR:HD1 | 5 | 0.24 |
| (2,673) | 1:127:A:GLY:H | 1:128:A:TYR:HD2 | 5 | 0.24 |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H | 5 | 0.24 |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H | 5 | 0.24 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 4 | 0.24 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 8 | 0.24 |
| (2,253) | 1:47:A:ALA:H | 1:48:A:ILE:HD11 | 5 | 0.24 |
| (2,253) | 1:47:A:ALA:H | 1:48:A:ILE:HD12 | 5 | 0.24 |
| (2,253) | 1:47:A:ALA:H | 1:48:A:ILE:HD13 | 5 | 0.24 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 7 | 0.24 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 7 | 0.24 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 7 | 0.24 |
| (2,178) | 1:36:A:ALA:H | 1:37:A:GLY:H | 8 | 0.24 |
| (1,2177) | 1:157:A:LYS:H | 1:158:A:ALA:HA | 10 | 0.24 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 5 | 0.24 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 5 | 0.24 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 5 | 0.24 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 7 | 0.24 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 7 | 0.24 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 7 | 0.24 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 2 | 0.24 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 3 | 0.24 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 8 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 6 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 6 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 6 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 6 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 6 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 6 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 6 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 6 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 6 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 7 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 7 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 7 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 7 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 7 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 7 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 7 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 7 | 0.24 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 7 | 0.24 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD11 | 7 | 0.24 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD12 | 7 | 0.24 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD13 | 7 | 0.24 |
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2 | 7 | 0.24 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 8 | 0.24 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 8 | 0.24 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 8 | 0.24 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG21 | 1 | 0.24 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG22 | 1 | 0.24 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG23 | 1 | 0.24 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG21 | 2 | 0.24 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG22 | 2 | 0.24 |
| (1,1803) | 1:129:A:THR:HA | 1:129:A:THR:HG23 | 2 | 0.24 |
| (1,1800) | 1:128:A:TYR:HD1 | 1:129:A:THR:HG21 | 4 | 0.24 |
| (1,1800) | 1:128:A:TYR:HD1 | 1:129:A:THR:HG22 | 4 | 0.24 |
| (1,1800) | 1:128:A:TYR:HD1 | 1:129:A:THR:HG23 | 4 | 0.24 |
| (1,1800) | 1:128:A:TYR:HD2 | 1:129:A:THR:HG21 | 4 | 0.24 |
| (1,1800) | 1:128:A:TYR:HD2 | 1:129:A:THR:HG22 | 4 | 0.24 |
| (1,1800) | 1:128:A:TYR:HD2 | 1:129:A:THR:HG23 | 4 | 0.24 |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H | 6 | 0.24 |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H | 6 | 0.24 |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H | 6 | 0.24 |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H | 2 | 0.24 |
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H | 2 | 0.24 |
| (1,1635) | 1:111:A:ILE:HB | 1:111:A:ILE:H | 8 | 0.24 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 9 | 0.24 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 9 | 0.24 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 9 | 0.24 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 10 | 0.24 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 10 | 0.24 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 10 | 0.24 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 3 | 0.24 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 8 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 4 | 0.24 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 1 | 0.24 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 3 | 0.24 |
| (1,941) | 1:71:A:LYS:HA | 1:74:A:PHE:HD1 | 5 | 0.24 |
| (1,941) | 1:71:A:LYS:HA | 1:74:A:PHE:HD2 | 5 | 0.24 |
| (1,886) | 1:68:A:GLU:HA | 1:71:A:LYS:HD2 | 5 | 0.24 |
| (1,886) | 1:68:A:GLU:HA | 1:71:A:LYS:HD3 | 5 | 0.24 |
| (1,873) | 1:67:A:ALA:HB1 | 1:68:A:GLU:H | 3 | 0.24 |
| (1,873) | 1:67:A:ALA:HB2 | 1:68:A:GLU:H | 3 | 0.24 |
| (1,873) | 1:67:A:ALA:HB3 | 1:68:A:GLU:H | 3 | 0.24 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 8 | 0.24 |
| (1,833) | 1:66:A:ASN:HB3 | 1:66:A:ASN:HD22 | 9 | 0.24 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 5 | 0.24 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 8 | 0.24 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 8 | 0.24 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 8 | 0.24 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 8 | 0.24 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 8 | 0.24 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 8 | 0.24 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 8 | 0.24 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 8 | 0.24 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 8 | 0.24 |
| (1,728) | 1:62:A:VAL:HG21 | 1:62:A:VAL:H | 3 | 0.24 |
| (1,728) | 1:62:A:VAL:HG22 | 1:62:A:VAL:H | 3 | 0.24 |
| (1,728) | 1:62:A:VAL:HG23 | 1:62:A:VAL:H | 3 | 0.24 |
| (1,727) | 1:62:A:VAL:HG11 | 1:177:A:PHE:HE1 | 3 | 0.24 |
| (1,727) | 1:62:A:VAL:HG11 | 1:177:A:PHE:HE2 | 3 | 0.24 |
| (1,727) | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE1 | 3 | 0.24 |
| (1,727) | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE2 | 3 | 0.24 |
| (1,727) | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE1 | 3 | 0.24 |
| (1,727) | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE2 | 3 | 0.24 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 8 | 0.24 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 8 | 0.24 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 8 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 5 | 0.24 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 2 | 0.24 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 2 | 0.24 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 7 | 0.24 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 7 | 0.24 |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H | 8 | 0.24 |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H | 8 | 0.24 |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H | 8 | 0.24 |
| (1,475) | 1:48:A:ILE:HA | 1:151:A:VAL:HG21 | 5 | 0.24 |
| (1,475) | 1:48:A:ILE:HA | 1:151:A:VAL:HG22 | 5 | 0.24 |
| (1,475) | 1:48:A:ILE:HA | 1:151:A:VAL:HG23 | 5 | 0.24 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE1 | 4 | 0.24 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE2 | 4 | 0.24 |
| (1,392) | 1:44:A:ILE:HG21 | 1:158:A:ALA:H | 10 | 0.24 |
| (1,392) | 1:44:A:ILE:HG22 | 1:158:A:ALA:H | 10 | 0.24 |
| (1,392) | 1:44:A:ILE:HG23 | 1:158:A:ALA:H | 10 | 0.24 |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE1 | 2 | 0.24 |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE2 | 2 | 0.24 |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE1 | 2 | 0.24 |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE2 | 2 | 0.24 |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE1 | 2 | 0.24 |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE2 | 2 | 0.24 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 4 | 0.24 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 4 | 0.24 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 4 | 0.24 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 4 | 0.24 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 4 | 0.24 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 4 | 0.24 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 4 | 0.24 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 4 | 0.24 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 4 | 0.24 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 2 | 0.24 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 2 | 0.24 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 2 | 0.24 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 2 | 0.24 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 2 | 0.24 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 2 | 0.24 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 4 | 0.24 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 4 | 0.24 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 4 | 0.24 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 4 | 0.24 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 4 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 4 | 0.24 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 6 | 0.24 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 8 | 0.24 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG21 | 5 | 0.24 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG22 | 5 | 0.24 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG23 | 5 | 0.24 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 7 | 0.23 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD1 | 5 | 0.23 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD2 | 5 | 0.23 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD11 | 3 | 0.23 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD12 | 3 | 0.23 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD13 | 3 | 0.23 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 2 | 0.23 |
| (2,547) | 1:87:A:THR:HG21 | 1:91:A:ALA:H | 9 | 0.23 |
| (2,547) | 1:87:A:THR:HG22 | 1:91:A:ALA:H | 9 | 0.23 |
| (2,547) | 1:87:A:THR:HG23 | 1:91:A:ALA:H | 9 | 0.23 |
| (2,227) | 1:43:A:ASP:HB3 | 1:46:A:TYR:HE1 | 9 | 0.23 |
| (2,227) | 1:43:A:ASP:HB3 | 1:46:A:TYR:HE2 | 9 | 0.23 |
| (2,174) | 1:35:A:ALA:HB1 | 1:40:A:GLY:H | 5 | 0.23 |
| (2,174) | 1:35:A:ALA:HB2 | 1:40:A:GLY:H | 5 | 0.23 |
| (2,174) | 1:35:A:ALA:HB3 | 1:40:A:GLY:H | 5 | 0.23 |
| (2,4) | 1:15:A:THR:HG21 | 1:16:A:ALA:H | 5 | 0.23 |
| (2,4) | 1:15:A:THR:HG22 | 1:16:A:ALA:H | 5 | 0.23 |
| (2,4) | 1:15:A:THR:HG23 | 1:16:A:ALA:H | 5 | 0.23 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 10 | 0.23 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 10 | 0.23 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 10 | 0.23 |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H | 3 | 0.23 |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H | 3 | 0.23 |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H | 3 | 0.23 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 1 | 0.23 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 2 | 0.23 |
| (1,2321) | 1:171:A:LEU:HD11 | 1:171:A:LEU:H | 2 | 0.23 |
| (1,2321) | 1:171:A:LEU:HD12 | 1:171:A:LEU:H | 2 | 0.23 |
| (1,2321) | 1:171:A:LEU:HD13 | 1:171:A:LEU:H | 2 | 0.23 |
| (1,2310) | 1:170:A:SER:H | 1:171:A:LEU:HD11 | 2 | 0.23 |
| (1,2310) | 1:170:A:SER:H | 1:171:A:LEU:HD12 | 2 | 0.23 |
| (1,2310) | 1:170:A:SER:H | 1:171:A:LEU:HD13 | 2 | 0.23 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 10 | 0.23 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 10 | 0.23 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 10 | 0.23 |
| (1,2066) | 1:148:A:THR:HA | 1:149:A:LYS:H | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 2 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 3 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 10 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 10 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 10 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 10 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 10 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 10 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 10 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 10 | 0.23 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 10 | 0.23 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 8 | 0.23 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 8 | 0.23 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 8 | 0.23 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD11 | 3 | 0.23 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD12 | 3 | 0.23 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD13 | 3 | 0.23 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD11 | 9 | 0.23 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD12 | 9 | 0.23 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD13 | 9 | 0.23 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 5 | 0.23 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 5 | 0.23 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 5 | 0.23 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 6 | 0.23 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 6 | 0.23 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1978) | 1:139:A:PRO:HA | 1:142:A:ILE:HD11 | 1 | 0.23 |
| (1,1978) | 1:139:A:PRO:HA | 1:142:A:ILE:HD12 | 1 | 0.23 |
| (1,1978) | 1:139:A:PRO:HA | 1:142:A:ILE:HD13 | 1 | 0.23 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 4 | 0.23 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 4 | 0.23 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 4 | 0.23 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 7 | 0.23 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 7 | 0.23 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 7 | 0.23 |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H | 9 | 0.23 |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H | 9 | 0.23 |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H | 9 | 0.23 |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H | 1 | 0.23 |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H | 1 | 0.23 |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H | 1 | 0.23 |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H | 5 | 0.23 |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H | 5 | 0.23 |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H | 5 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD21 | 8 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD22 | 8 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD23 | 8 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD21 | 9 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD22 | 9 | 0.23 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD23 | 9 | 0.23 |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H | 4 | 0.23 |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H | 4 | 0.23 |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H | 4 | 0.23 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 1 | 0.23 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 1 | 0.23 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 1 | 0.23 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 5 | 0.23 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 5 | 0.23 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 5 | 0.23 |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 1 | 0.23 |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 1 | 0.23 |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 1 | 0.23 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 7 | 0.23 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 5 | 0.23 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 7 | 0.23 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 6 | 0.23 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 8 | 0.23 |
| (1,1038) | 1:74:A:PHE:HZ | 1:171:A:LEU:H | 8 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 4 | 0.23 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 5 | 0.23 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 6 | 0.23 |
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 7 | 0.23 |
| (1,915) | 1:69:A:GLN:HG3 | 1:70:A:LEU:H | 6 | 0.23 |
| (1,915) | 1:69:A:GLN:HG3 | 1:70:A:LEU:H | 9 | 0.23 |
| (1,911) | 1:69:A:GLN:HE22 | 1:70:A:LEU:H | 9 | 0.23 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 10 | 0.23 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 10 | 0.23 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 10 | 0.23 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 10 | 0.23 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 10 | 0.23 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 10 | 0.23 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 10 | 0.23 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 10 | 0.23 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 10 | 0.23 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 2 | 0.23 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 2 | 0.23 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 2 | 0.23 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 1 | 0.23 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 1 | 0.23 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 3 | 0.23 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 3 | 0.23 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 4 | 0.23 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 4 | 0.23 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 5 | 0.23 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 5 | 0.23 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 8 | 0.23 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 8 | 0.23 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 9 | 0.23 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 9 | 0.23 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 10 | 0.23 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 10 | 0.23 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 5 | 0.23 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 5 | 0.23 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 5 | 0.23 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 5 | 0.23 |
| (1,498) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HZ2 | 5 | 0.23 |
| (1,498) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HZ2 | 5 | 0.23 |
| (1,498) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HZ2 | 5 | 0.23 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 3 | 0.23 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,455) | 1:47:A:ALA:HB1 | 1:48:A:ILE:H | 4 | 0.23 |
| (1,455) | 1:47:A:ALA:HB2 | 1:48:A:ILE:H | 4 | 0.23 |
| (1,455) | 1:47:A:ALA:HB3 | 1:48:A:ILE:H | 4 | 0.23 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 10 | 0.23 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 10 | 0.23 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 10 | 0.23 |
| (1,246) | 1:32:A:ILE:HG21 | 1:168:A:PHE:HE1 | 10 | 0.23 |
| (1,246) | 1:32:A:ILE:HG21 | 1:168:A:PHE:HE2 | 10 | 0.23 |
| (1,246) | 1:32:A:ILE:HG22 | 1:168:A:PHE:HE1 | 10 | 0.23 |
| (1,246) | 1:32:A:ILE:HG22 | 1:168:A:PHE:HE2 | 10 | 0.23 |
| (1,246) | 1:32:A:ILE:HG23 | 1:168:A:PHE:HE1 | 10 | 0.23 |
| (1,246) | 1:32:A:ILE:HG23 | 1:168:A:PHE:HE2 | 10 | 0.23 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 10 | 0.23 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG21 | 10 | 0.23 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG22 | 10 | 0.23 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG23 | 10 | 0.23 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE1 | 4 | 0.22 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE2 | 4 | 0.22 |
| (2,714) | 1:141:A:LYS:HD2 | 1:142:A:ILE:H | 9 | 0.22 |
| (2,714) | 1:141:A:LYS:HD3 | 1:142:A:ILE:H | 9 | 0.22 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG2 | 7 | 0.22 |
| (2,593) | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG3 | 7 | 0.22 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD11 | 1 | 0.22 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD12 | 1 | 0.22 |
| (2,590) | 1:110:A:VAL:H | 1:111:A:ILE:HD13 | 1 | 0.22 |
| (2,537) | 1:85:A:TYR:H | 1:85:A:TYR:HE1 | 2 | 0.22 |
| (2,537) | 1:85:A:TYR:H | 1:85:A:TYR:HE2 | 2 | 0.22 |
| (2,525) | 1:85:A:TYR:HE1 | 1:85:A:TYR:H | 2 | 0.22 |
| (2,525) | 1:85:A:TYR:HE2 | 1:85:A:TYR:H | 2 | 0.22 |
| (2,488) | 1:80:A:GLN:H | 1:81:A:ILE:HD11 | 4 | 0.22 |
| (2,488) | 1:80:A:GLN:H | 1:81:A:ILE:HD12 | 4 | 0.22 |
| (2,488) | 1:80:A:GLN:H | 1:81:A:ILE:HD13 | 4 | 0.22 |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H | 10 | 0.22 |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H | 10 | 0.22 |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H | 10 | 0.22 |
| (1,2425) | 1:177:A:PHE:HD1 | 1:177:A:PHE:H | 1 | 0.22 |
| (1,2425) | 1:177:A:PHE:HD2 | 1:177:A:PHE:H | 1 | 0.22 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 10 | 0.22 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 10 | 0.22 |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 10 | 0.22 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 7 | 0.22 |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H | 8 | 0.22 |
| (1,2154) | 1:156:A:PHE:HD1 | 1:156:A:PHE:H | 9 | 0.22 |
| (1,2154) | 1:156:A:PHE:HD2 | 1:156:A:PHE:H | 9 | 0.22 |
| (1,2154) | 1:156:A:PHE:HD1 | 1:156:A:PHE:H | 10 | 0.22 |
| (1,2154) | 1:156:A:PHE:HD2 | 1:156:A:PHE:H | 10 | 0.22 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 3 | 0.22 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 3 | 0.22 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 3 | 0.22 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG21 | 6 | 0.22 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG22 | 6 | 0.22 |
| (1,2093) | 1:153:A:ILE:HA | 1:153:A:ILE:HG23 | 6 | 0.22 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG21 | 4 | 0.22 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 4 | 0.22 |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 4 | 0.22 |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H | 5 | 0.22 |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H | 5 | 0.22 |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H | 5 | 0.22 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG21 | 1 | 0.22 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG22 | 1 | 0.22 |
| (1,2003) | 1:142:A:ILE:HA | 1:142:A:ILE:HG23 | 1 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 1 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 1 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 1 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 3 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 3 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 3 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 5 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 5 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 5 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 10 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 10 | 0.22 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 10 | 0.22 |
| (1,1845) | 1:132:A:SER:HB2 | 1:145:A:TYR:HD1 | 9 | 0.22 |
| (1,1845) | 1:132:A:SER:HB2 | 1:145:A:TYR:HD2 | 9 | 0.22 |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H | 3 | 0.22 |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H | 3 | 0.22 |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H | 3 | 0.22 |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H | 9 | 0.22 |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H | 9 | 0.22 |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H | 9 | 0.22 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD21 | 3 | 0.22 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD22 | 3 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD23 | 3 | 0.22 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 2 | 0.22 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 5 | 0.22 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 9 | 0.22 |
| (1,1446) | 1:90:A:THR:HA | 1:93:A:GLY:H | 9 | 0.22 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG21 | 2 | 0.22 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG22 | 2 | 0.22 |
| (1,1445) | 1:90:A:THR:HA | 1:90:A:THR:HG23 | 2 | 0.22 |
| (1,1400) | 1:87:A:THR:HG21 | 1:88:A:ASN:HA | 9 | 0.22 |
| (1,1400) | 1:87:A:THR:HG22 | 1:88:A:ASN:HA | 9 | 0.22 |
| (1,1400) | 1:87:A:THR:HG23 | 1:88:A:ASN:HA | 9 | 0.22 |
| (1,1338) | 1:85:A:TYR:HD1 | 1:86:A:GLU:H | 8 | 0.22 |
| (1,1338) | 1:85:A:TYR:HD2 | 1:86:A:GLU:H | 8 | 0.22 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD21 | 7 | 0.22 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD22 | 7 | 0.22 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD23 | 7 | 0.22 |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H | 4 | 0.22 |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H | 4 | 0.22 |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H | 4 | 0.22 |
| (1,1185) | 1:80:A:GLN:HB2 | 1:159:A:PHE:HD1 | 7 | 0.22 |
| (1,1185) | 1:80:A:GLN:HB2 | 1:159:A:PHE:HD2 | 7 | 0.22 |
| (1,1185) | 1:80:A:GLN:HB3 | 1:159:A:PHE:HD1 | 7 | 0.22 |
| (1,1185) | 1:80:A:GLN:HB3 | 1:159:A:PHE:HD2 | 7 | 0.22 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 2 | 0.22 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 6 | 0.22 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 4 | 0.22 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 10 | 0.22 |
| (1,1109) | 1:78:A:GLN:HA | 1:78:A:GLN:HG2 | 10 | 0.22 |
| (1,1109) | 1:78:A:GLN:HA | 1:78:A:GLN:HG3 | 10 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 3 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 3 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 7 | 0.22 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 7 | 0.22 |
| (1,1020) | 1:74:A:PHE:HD1 | 1:162:A:ALA:HA | 9 | 0.22 |
| (1,1020) | 1:74:A:PHE:HD2 | 1:162:A:ALA:HA | 9 | 0.22 |
| (1,911) | 1:69:A:GLN:HE22 | 1:70:A:LEU:H | 5 | 0.22 |
| (1,909) | 1:69:A:GLN:HB2 | 1:70:A:LEU:H | 6 | 0.22 |
| (1,873) | 1:67:A:ALA:HB1 | 1:68:A:GLU:H | 5 | 0.22 |
| (1,873) | 1:67:A:ALA:HB2 | 1:68:A:GLU:H | 5 | 0.22 |
| (1,873) | 1:67:A:ALA:HB3 | 1:68:A:GLU:H | 5 | 0.22 |
| (1,728) | 1:62:A:VAL:HG21 | 1:62:A:VAL:H | 5 | 0.22 |
| (1,728) | 1:62:A:VAL:HG22 | 1:62:A:VAL:H | 5 | 0.22 |
| (1,728) | 1:62:A:VAL:HG23 | 1:62:A:VAL:H | 5 | 0.22 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 10 | 0.22 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 10 | 0.22 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 10 | 0.22 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 7 | 0.22 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 4 | 0.22 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 7 | 0.22 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 7 | 0.22 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 7 | 0.22 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 1 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 1 | 0.22 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 1 | 0.22 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 8 | 0.22 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 8 | 0.22 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 8 | 0.22 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 5 | 0.22 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 10 | 0.22 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 10 | 0.22 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 10 | 0.22 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 10 | 0.22 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 10 | 0.22 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG21 | 3 | 0.22 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG22 | 3 | 0.22 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG23 | 3 | 0.22 |
| (1,289) | 1:37:A:GLY:HA3 | 1:37:A:GLY:H | 7 | 0.22 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 2 | 0.21 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE1 | 1 | 0.21 |
| (2,768) | 1:173:A:VAL:HB | 1:175:A:PHE:HE2 | 1 | 0.21 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD1 | 9 | 0.21 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD2 | 9 | 0.21 |
| (2,714) | 1:141:A:LYS:HD2 | 1:142:A:ILE:H | 3 | 0.21 |
| (2,714) | 1:141:A:LYS:HD3 | 1:142:A:ILE:H | 3 | 0.21 |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H | 9 | 0.21 |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H | 9 | 0.21 |
| (2,618) | 1:119:A:ALA:HB1 | 1:149:A:LYS:H | 3 | 0.21 |
| (2,618) | 1:119:A:ALA:HB2 | 1:149:A:LYS:H | 3 | 0.21 |
| (2,618) | 1:119:A:ALA:HB3 | 1:149:A:LYS:H | 3 | 0.21 |
| (2,552) | 1:87:A:THR:H | 1:92:A:LEU:HB2 | 9 | 0.21 |
| (2,468) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HE1 | 3 | 0.21 |
| (2,468) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HE2 | 3 | 0.21 |
| (2,468) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HE1 | 3 | 0.21 |
| (2,468) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HE2 | 3 | 0.21 |
| (2,468) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HE1 | 3 | 0.21 |
| (2,468) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HE2 | 3 | 0.21 |
| (2,341) | 1:59:A:LYS:H | 1:59:A:LYS:HE2 | 5 | 0.21 |
| (2,341) | 1:59:A:LYS:H | 1:59:A:LYS:HE3 | 5 | 0.21 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 10 | 0.21 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 10 | 0.21 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 10 | 0.21 |
| (2,178) | 1:36:A:ALA:H | 1:37:A:GLY:H | 4 | 0.21 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 8 | 0.21 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 8 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 8 | 0.21 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 7 | 0.21 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 7 | 0.21 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 7 | 0.21 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 7 | 0.21 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 7 | 0.21 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 7 | 0.21 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 8 | 0.21 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG21 | 2 | 0.21 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG22 | 2 | 0.21 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG23 | 2 | 0.21 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG21 | 7 | 0.21 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG22 | 7 | 0.21 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG23 | 7 | 0.21 |
| (1,2154) | 1:156:A:PHE:HD1 | 1:156:A:PHE:H | 2 | 0.21 |
| (1,2154) | 1:156:A:PHE:HD2 | 1:156:A:PHE:H | 2 | 0.21 |
| (1,2154) | 1:156:A:PHE:HD1 | 1:156:A:PHE:H | 8 | 0.21 |
| (1,2154) | 1:156:A:PHE:HD2 | 1:156:A:PHE:H | 8 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 9 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 9 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 9 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 9 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 9 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 9 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 9 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 9 | 0.21 |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 9 | 0.21 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD11 | 6 | 0.21 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD12 | 6 | 0.21 |
| (1,2021) | 1:143:A:ILE:HA | 1:143:A:ILE:HD13 | 6 | 0.21 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 5 | 0.21 |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB | 6 | 0.21 |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB | 6 | 0.21 |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB | 6 | 0.21 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 9 | 0.21 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 9 | 0.21 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 9 | 0.21 |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H | 1 | 0.21 |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H | 1 | 0.21 |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H | 1 | 0.21 |
| (1,1775) | 1:121:A:LEU:HB2 | 1:121:A:LEU:H | 9 | 0.21 |
| (1,1774) | 1:121:A:LEU:HB3 | 1:121:A:LEU:H | 6 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1770) | 1:120:A:VAL:HG21 | 1:121:A:LEU:H | 7 | 0.21 |
| (1,1770) | 1:120:A:VAL:HG22 | 1:121:A:LEU:H | 7 | 0.21 |
| (1,1770) | 1:120:A:VAL:HG23 | 1:121:A:LEU:H | 7 | 0.21 |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H | 8 | 0.21 |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H | 8 | 0.21 |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H | 8 | 0.21 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD21 | 2 | 0.21 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD22 | 2 | 0.21 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD23 | 2 | 0.21 |
| (1,1635) | 1:111:A:ILE:HB | 1:111:A:ILE:H | 6 | 0.21 |
| (1,1505) | 1:98:A:THR:HA | 1:100:A:ALA:H | 3 | 0.21 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 1 | 0.21 |
| (1,1459) | 1:92:A:LEU:HG | 1:92:A:LEU:H | 4 | 0.21 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 1 | 0.21 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 1 | 0.21 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 1 | 0.21 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 3 | 0.21 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 3 | 0.21 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 3 | 0.21 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 6 | 0.21 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 6 | 0.21 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 6 | 0.21 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 8 | 0.21 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 1 | 0.21 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 9 | 0.21 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 7 | 0.21 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 1 | 0.21 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 5 | 0.21 |
| (1,915) | 1:69:A:GLN:HG3 | 1:70:A:LEU:H | 2 | 0.21 |
| (1,912) | 1:69:A:GLN:HG3 | 1:69:A:GLN:HE21 | 9 | 0.21 |
| (1,873) | 1:67:A:ALA:HB1 | 1:68:A:GLU:H | 9 | 0.21 |
| (1,873) | 1:67:A:ALA:HB2 | 1:68:A:GLU:H | 9 | 0.21 |
| (1,873) | 1:67:A:ALA:HB3 | 1:68:A:GLU:H | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 9 | 0.21 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 9 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 9 | 0.21 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 9 | 0.21 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 9 | 0.21 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 9 | 0.21 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 9 | 0.21 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 9 | 0.21 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 6 | 0.21 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 6 | 0.21 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 6 | 0.21 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 4 | 0.21 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 8 | 0.21 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 7 | 0.21 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 2 | 0.21 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 2 | 0.21 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 2 | 0.21 |
| (1,296) | 1:38:A:ALA:HB1 | 1:39:A:GLN:H | 8 | 0.21 |
| (1,296) | 1:38:A:ALA:HB2 | 1:39:A:GLN:H | 8 | 0.21 |
| (1,296) | 1:38:A:ALA:HB3 | 1:39:A:GLN:H | 8 | 0.21 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 7 | 0.21 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 7 | 0.21 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 7 | 0.21 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 7 | 0.21 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 9 | 0.21 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 9 | 0.21 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 2 | 0.21 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 5 | 0.21 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 9 | 0.21 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 2 | 0.2 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 4 | 0.2 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 6 | 0.2 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 8 | 0.2 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 9 | 0.2 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 10 | 0.2 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 4 | 0.2 |
| (3,2) | 1:33:A:THR:HA | 1:34:A:PRO:HD3 | 2 | 0.2 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 1 | 0.2 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 1 | 0.2 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 1 | 0.2 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 10 | 0.2 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 10 | 0.2 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 10 | 0.2 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 1 | 0.2 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 1 | 0.2 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 10 | 0.2 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 10 | 0.2 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 10 | 0.2 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE1 | 9 | 0.2 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE2 | 9 | 0.2 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD11 | 8 | 0.2 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD12 | 8 | 0.2 |
| (2,729) | 1:151:A:VAL:H | 1:153:A:ILE:HD13 | 8 | 0.2 |
| (2,726) | 1:145:A:TYR:HE1 | 1:145:A:TYR:H | 5 | 0.2 |
| (2,726) | 1:145:A:TYR:HE2 | 1:145:A:TYR:H | 5 | 0.2 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 3 | 0.2 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 3 | 0.2 |
| (2,298) | 1:54:A:GLN:HB3 | 1:54:A:GLN:HE21 | 5 | 0.2 |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H | 10 | 0.2 |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H | 10 | 0.2 |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H | 10 | 0.2 |
| (1,2348) | 1:173:A:VAL:HB | 1:173:A:VAL:H | 6 | 0.2 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 2 | 0.2 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 2 | 0.2 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 2 | 0.2 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 6 | 0.2 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 6 | 0.2 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 6 | 0.2 |
| (1,2260) | 1:163:A:LYS:H | 1:168:A:PHE:HZ | 1 | 0.2 |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H | 7 | 0.2 |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H | 7 | 0.2 |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H | 7 | 0.2 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 2 | 0.2 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 9 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 1 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 2 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 3 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 4 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 5 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 6 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 7 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 8 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 9 | 0.2 |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2 | 10 | 0.2 |
| (1,1774) | 1:121:A:LEU:HB3 | 1:121:A:LEU:H | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1723) | 1:116:A:GLU:HG2 | 1:116:A:GLU:H | 2 | 0.2 |
| (1,1723) | 1:116:A:GLU:HG3 | 1:116:A:GLU:H | 2 | 0.2 |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H | 2 | 0.2 |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H | 2 | 0.2 |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H | 2 | 0.2 |
| (1,1572) | 1:104:A:LEU:HD11 | 1:104:A:LEU:H | 4 | 0.2 |
| (1,1572) | 1:104:A:LEU:HD12 | 1:104:A:LEU:H | 4 | 0.2 |
| (1,1572) | 1:104:A:LEU:HD13 | 1:104:A:LEU:H | 4 | 0.2 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 6 | 0.2 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 6 | 0.2 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 6 | 0.2 |
| (1,1371) | 1:86:A:GLU:H | 1:134:A:TRP:HE1 | 7 | 0.2 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 4 | 0.2 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 4 | 0.2 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 4 | 0.2 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 3 | 0.2 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 4 | 0.2 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 3 | 0.2 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 8 | 0.2 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 2 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 10 | 0.2 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 10 | 0.2 |
| (1,1019) | 1:74:A:PHE:HD1 | 1:160:A:TYR:HD1 | 7 | 0.2 |
| (1,1019) | 1:74:A:PHE:HD1 | 1:160:A:TYR:HD2 | 7 | 0.2 |
| (1,1019) | 1:74:A:PHE:HD2 | 1:160:A:TYR:HD1 | 7 | 0.2 |
| (1,1019) | 1:74:A:PHE:HD2 | 1:160:A:TYR:HD2 | 7 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1013) | 1:74:A:PHE:HB2 | 1:163:A:LYS:H | 9 | 0.2 |
| (1,941) | 1:71:A:LYS:HA | 1:74:A:PHE:HD1 | 1 | 0.2 |
| (1,941) | 1:71:A:LYS:HA | 1:74:A:PHE:HD2 | 1 | 0.2 |
| (1,914) | 1:69:A:GLN:HG3 | 1:69:A:GLN:H | 1 | 0.2 |
| (1,914) | 1:69:A:GLN:HG3 | 1:69:A:GLN:H | 7 | 0.2 |
| (1,909) | 1:69:A:GLN:HB2 | 1:70:A:LEU:H | 10 | 0.2 |
| (1,908) | 1:69:A:GLN:HB3 | 1:70:A:LEU:H | 8 | 0.2 |
| (1,894) | 1:68:A:GLU:H | 1:69:A:GLN:H | 4 | 0.2 |
| (1,857) | 1:66:A:ASN:HD22 | 1:174:A:ILE:H | 7 | 0.2 |
| (1,849) | 1:66:A:ASN:HD22 | 1:66:A:ASN:H | 10 | 0.2 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 1 | 0.2 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 1 | 0.2 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 1 | 0.2 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 1 | 0.2 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 1 | 0.2 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 1 | 0.2 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 1 | 0.2 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 1 | 0.2 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 1 | 0.2 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG11 | 6 | 0.2 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG12 | 6 | 0.2 |
| (1,709) | 1:62:A:VAL:HA | 1:62:A:VAL:HG13 | 6 | 0.2 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 6 | 0.2 |
| (1,647) | 1:58:A:VAL:HB | 1:58:A:VAL:H | 5 | 0.2 |
| (1,647) | 1:58:A:VAL:HB | 1:58:A:VAL:H | 6 | 0.2 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG21 | 4 | 0.2 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG22 | 4 | 0.2 |
| (1,621) | 1:55:A:VAL:H | 1:55:A:VAL:HG23 | 4 | 0.2 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 8 | 0.2 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 8 | 0.2 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 8 | 0.2 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG21 | 5 | 0.2 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG22 | 5 | 0.2 |
| (1,556) | 1:50:A:TRP:HD1 | 1:151:A:VAL:HG23 | 5 | 0.2 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 8 | 0.2 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 10 | 0.2 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 9 | 0.2 |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1 | 2 | 0.2 |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1 | 2 | 0.2 |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1 | 2 | 0.2 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE1 | 1 | 0.2 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE2 | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,392) | 1:44:A:ILE:HG21 | 1:158:A:ALA:H | 8 | 0.2 |
| (1,392) | 1:44:A:ILE:HG22 | 1:158:A:ALA:H | 8 | 0.2 |
| (1,392) | 1:44:A:ILE:HG23 | 1:158:A:ALA:H | 8 | 0.2 |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H | 1 | 0.2 |
| (1,235) | 1:32:A:ILE:HG22 | 1:33:A:THR:H | 1 | 0.2 |
| (1,235) | 1:32:A:ILE:HG23 | 1:33:A:THR:H | 1 | 0.2 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE1 | 1 | 0.2 |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE2 | 1 | 0.2 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE1 | 1 | 0.2 |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE2 | 1 | 0.2 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE1 | 1 | 0.2 |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE2 | 1 | 0.2 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 3 | 0.2 |
| (1,11) | 1:20:A:SER:HB2 | 1:21:A:GLU:H | 7 | 0.2 |
| (1,11) | 1:20:A:SER:HB3 | 1:21:A:GLU:H | 7 | 0.2 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 1 | 0.19 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 3 | 0.19 |
| (2,714) | 1:141:A:LYS:HD2 | 1:142:A:ILE:H | 4 | 0.19 |
| (2,714) | 1:141:A:LYS:HD3 | 1:142:A:ILE:H | 4 | 0.19 |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H | 6 | 0.19 |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H | 6 | 0.19 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 7 | 0.19 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 7 | 0.19 |
| (2,534) | 1:85:A:TYR:HE1 | 1:151:A:VAL:H | 10 | 0.19 |
| (2,534) | 1:85:A:TYR:HE2 | 1:151:A:VAL:H | 10 | 0.19 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD21 | 7 | 0.19 |
| (2,239) | 1:46:A:TYR:HB3 | 1:155:A:ASN:HD22 | 7 | 0.19 |
| (2,176) | 1:35:A:ALA:H | 1:37:A:GLY:H | 7 | 0.19 |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H | 2 | 0.19 |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H | 2 | 0.19 |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H | 2 | 0.19 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 4 | 0.19 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 4 | 0.19 |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 4 | 0.19 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 2 | 0.19 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 2 | 0.19 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 2 | 0.19 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 6 | 0.19 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 6 | 0.19 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 6 | 0.19 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 8 | 0.19 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 8 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 8 | 0.19 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 1 | 0.19 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 1 | 0.19 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 1 | 0.19 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 7 | 0.19 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 7 | 0.19 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 7 | 0.19 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG21 | 9 | 0.19 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG22 | 9 | 0.19 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG23 | 9 | 0.19 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD11 | 9 | 0.19 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD12 | 9 | 0.19 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD13 | 9 | 0.19 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 1 | 0.19 |
| (1,2091) | 1:152:A:ALA:H | 1:153:A:ILE:HD11 | 3 | 0.19 |
| (1,2091) | 1:152:A:ALA:H | 1:153:A:ILE:HD12 | 3 | 0.19 |
| (1,2091) | 1:152:A:ALA:H | 1:153:A:ILE:HD13 | 3 | 0.19 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 1 | 0.19 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 1 | 0.19 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 1 | 0.19 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 2 | 0.19 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 2 | 0.19 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 2 | 0.19 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 7 | 0.19 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 7 | 0.19 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 7 | 0.19 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 7 | 0.19 |
| (1,1882) | 1:134:A:TRP:HA | 1:143:A:ILE:HA | 4 | 0.19 |
| (1,1882) | 1:134:A:TRP:HA | 1:143:A:ILE:HA | 8 | 0.19 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 2 | 0.19 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 2 | 0.19 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 2 | 0.19 |
| (1,1835) | 1:132:A:SER:HA | 1:145:A:TYR:HB2 | 6 | 0.19 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG21 | 4 | 0.19 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG22 | 4 | 0.19 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG23 | 4 | 0.19 |
| (1,1775) | 1:121:A:LEU:HB2 | 1:121:A:LEU:H | 2 | 0.19 |
| (1,1774) | 1:121:A:LEU:HB3 | 1:121:A:LEU:H | 4 | 0.19 |
| (1,1635) | 1:111:A:ILE:HB | 1:111:A:ILE:H | 7 | 0.19 |
| (1,1505) | 1:98:A:THR:HA | 1:100:A:ALA:H | 6 | 0.19 |
| (1,1505) | 1:98:A:THR:HA | 1:100:A:ALA:H | 7 | 0.19 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 3 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 4 | 0.19 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 6 | 0.19 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 8 | 0.19 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 10 | 0.19 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 8 | 0.19 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 8 | 0.19 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 8 | 0.19 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 1 | 0.19 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 1 | 0.19 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 1 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB1 | 2 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB2 | 2 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB3 | 2 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB1 | 2 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB2 | 2 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB3 | 2 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB1 | 2 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB2 | 2 | 0.19 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB3 | 2 | 0.19 |
| (1,1173) | 1:79:A:ILE:H | 1:158:A:ALA:HA | 1 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 7 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 7 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 7 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 7 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 7 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 7 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 7 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 7 | 0.19 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 7 | 0.19 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 2 | 0.19 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 6 | 0.19 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 5 | 0.19 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 6 | 0.19 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 9 | 0.19 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 10 | 0.19 |
| (1,1095) | 1:77:A:LEU:HD11 | 1:159:A:PHE:H | 6 | 0.19 |
| (1,1095) | 1:77:A:LEU:HD12 | 1:159:A:PHE:H | 6 | 0.19 |
| (1,1095) | 1:77:A:LEU:HD13 | 1:159:A:PHE:H | 6 | 0.19 |
| (1,1095) | 1:77:A:LEU:HD21 | 1:159:A:PHE:H | 6 | 0.19 |
| (1,1095) | 1:77:A:LEU:HD22 | 1:159:A:PHE:H | 6 | 0.19 |
| (1,1095) | 1:77:A:LEU:HD23 | 1:159:A:PHE:H | 6 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 1 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 2 | 0.19 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 2 | 0.19 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 8 | 0.19 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 9 | 0.19 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD21 | 9 | 0.19 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD22 | 9 | 0.19 |
| (1,992) | 1:73:A:TYR:HE1 | 1:171:A:LEU:HD23 | 9 | 0.19 |
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD21 | 9 | 0.19 |
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD22 | 9 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,992) | 1:73:A:TYR:HE2 | 1:171:A:LEU:HD23 | 9 | 0.19 |
| (1,989) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HE1 | 2 | 0.19 |
| (1,989) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HE2 | 2 | 0.19 |
| (1,989) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HE1 | 2 | 0.19 |
| (1,989) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HE2 | 2 | 0.19 |
| (1,915) | 1:69:A:GLN:HG3 | 1:70:A:LEU:H | 8 | 0.19 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 5 | 0.19 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 7 | 0.19 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 7 | 0.19 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 7 | 0.19 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 7 | 0.19 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 7 | 0.19 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 7 | 0.19 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 7 | 0.19 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 7 | 0.19 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 7 | 0.19 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 10 | 0.19 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 10 | 0.19 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 10 | 0.19 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 8 | 0.19 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 8 | 0.19 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 8 | 0.19 |
| (1,647) | 1:58:A:VAL:HB | 1:58:A:VAL:H | 3 | 0.19 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 10 | 0.19 |
| (1,598) | 1:53:A:ASP:H | 1:54:A:GLN:H | 5 | 0.19 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 2 | 0.19 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 2 | 0.19 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 2 | 0.19 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 1 | 0.19 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 1 | 0.19 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 2 | 0.19 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 3 | 0.19 |
| (1,543) | 1:50:A:TRP:HA | 1:151:A:VAL:HA | 8 | 0.19 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 6 | 0.19 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 6 | 0.19 |
| (1,445) | 1:46:A:TYR:HE1 | 1:141:A:LYS:HE3 | 4 | 0.19 |
| (1,445) | 1:46:A:TYR:HE2 | 1:141:A:LYS:HE3 | 4 | 0.19 |
| (1,292) | 1:37:A:GLY:HA2 | 1:37:A:GLY:H | 4 | 0.19 |
| (1,260) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD3 | 4 | 0.19 |
| (1,260) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD3 | 4 | 0.19 |
| (1,260) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD3 | 4 | 0.19 |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H | 5 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,235) | 1:32:A:ILE:HG22 | 1:33:A:THR:H | 5 | 0.19 |
| (1,235) | 1:32:A:ILE:HG23 | 1:33:A:THR:H | 5 | 0.19 |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H | 6 | 0.19 |
| (1,235) | 1:32:A:ILE:HG22 | 1:33:A:THR:H | 6 | 0.19 |
| (1,235) | 1:32:A:ILE:HG23 | 1:33:A:THR:H | 6 | 0.19 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 3 | 0.19 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 3 | 0.19 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 3 | 0.19 |
| (1,109) | 1:26:A:GLU:H | 1:47:A:ALA:HA | 7 | 0.19 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 1 | 0.19 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 7 | 0.19 |
| (1,77) | 1:25:A:VAL:HG11 | 1:25:A:VAL:H | 6 | 0.19 |
| (1,77) | 1:25:A:VAL:HG12 | 1:25:A:VAL:H | 6 | 0.19 |
| (1,77) | 1:25:A:VAL:HG13 | 1:25:A:VAL:H | 6 | 0.19 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 1 | 0.18 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 2 | 0.18 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 3 | 0.18 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 4 | 0.18 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 8 | 0.18 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 9 | 0.18 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 10 | 0.18 |
| (2,760) | 1:168:A:PHE:HE1 | 1:171:A:LEU:HG | 1 | 0.18 |
| (2,760) | 1:168:A:PHE:HE2 | 1:171:A:LEU:HG | 1 | 0.18 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE1 | 1 | 0.18 |
| (2,740) | 1:162:A:ALA:HA | 1:168:A:PHE:HE2 | 1 | 0.18 |
| (2,723) | 1:145:A:TYR:HA | 1:147:A:GLU:HG2 | 6 | 0.18 |
| (2,723) | 1:145:A:TYR:HA | 1:147:A:GLU:HG3 | 6 | 0.18 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE1 | 5 | 0.18 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE2 | 5 | 0.18 |
| (2,352) | 1:63:A:THR:H | 1:175:A:PHE:HE1 | 6 | 0.18 |
| (2,352) | 1:63:A:THR:H | 1:175:A:PHE:HE2 | 6 | 0.18 |
| (2,194) | 1:38:A:ALA:HB1 | 1:39:A:GLN:HE21 | 8 | 0.18 |
| (2,194) | 1:38:A:ALA:HB2 | 1:39:A:GLN:HE21 | 8 | 0.18 |
| (2,194) | 1:38:A:ALA:HB3 | 1:39:A:GLN:HE21 | 8 | 0.18 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 5 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 1 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 1 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 1 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 3 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 3 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 3 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 4 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 4 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 4 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 5 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 5 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 5 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 7 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 7 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 7 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 10 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 10 | 0.18 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 10 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 3 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 3 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 3 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 4 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 4 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 4 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 5 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 5 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 5 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 8 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 8 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 8 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 10 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 10 | 0.18 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 10 | 0.18 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG21 | 1 | 0.18 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG22 | 1 | 0.18 |
| (1,2343) | 1:173:A:VAL:HA | 1:173:A:VAL:HG23 | 1 | 0.18 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD11 | 9 | 0.18 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD12 | 9 | 0.18 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD13 | 9 | 0.18 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD11 | 2 | 0.18 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD12 | 2 | 0.18 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD13 | 2 | 0.18 |
| (1,2272) | 1:166:A:MET:HB2 | 1:167:A:LEU:H | 10 | 0.18 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 4 | 0.18 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 4 | 0.18 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 4 | 0.18 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 4 | 0.18 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 4 | 0.18 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 4 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 3 | 0.18 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 10 | 0.18 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG21 | 6 | 0.18 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG22 | 6 | 0.18 |
| (1,1852) | 1:133:A:ILE:HA | 1:133:A:ILE:HG23 | 6 | 0.18 |
| (1,1774) | 1:121:A:LEU:HB3 | 1:121:A:LEU:H | 1 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB1 | 1:133:A:ILE:HD11 | 5 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB1 | 1:133:A:ILE:HD12 | 5 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB1 | 1:133:A:ILE:HD13 | 5 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB2 | 1:133:A:ILE:HD11 | 5 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB2 | 1:133:A:ILE:HD12 | 5 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB2 | 1:133:A:ILE:HD13 | 5 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB3 | 1:133:A:ILE:HD11 | 5 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB3 | 1:133:A:ILE:HD12 | 5 | 0.18 |
| (1,1757) | 1:119:A:ALA:HB3 | 1:133:A:ILE:HD13 | 5 | 0.18 |
| (1,1502) | 1:97:A:GLU:H | 1:98:A:THR:HA | 7 | 0.18 |
| (1,1483) | 1:95:A:PHE:HE1 | 1:116:A:GLU:HB3 | 8 | 0.18 |
| (1,1483) | 1:95:A:PHE:HE2 | 1:116:A:GLU:HB3 | 8 | 0.18 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 3 | 0.18 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 3 | 0.18 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 3 | 0.18 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 9 | 0.18 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 9 | 0.18 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 9 | 0.18 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG21 | 4 | 0.18 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG22 | 4 | 0.18 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG23 | 4 | 0.18 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD21 | 3 | 0.18 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD22 | 3 | 0.18 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD23 | 3 | 0.18 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD21 | 8 | 0.18 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD22 | 8 | 0.18 |
| (1,1298) | 1:83:A:SER:HA | 1:154:A:LEU:HD23 | 8 | 0.18 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG21 | 8 | 0.18 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG22 | 8 | 0.18 |
| (1,1252) | 1:82:A:THR:HA | 1:82:A:THR:HG23 | 8 | 0.18 |
| (1,1180) | 1:80:A:GLN:HA | 1:101:A:VAL:H | 5 | 0.18 |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H | 5 | 0.18 |
| (1,1128) | 1:78:A:GLN:H | 1:158:A:ALA:HA | 8 | 0.18 |
| (1,1128) | 1:78:A:GLN:H | 1:158:A:ALA:HA | 10 | 0.18 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 2 | 0.18 |
| (1,1114) | 1:78:A:GLN:HA | 1:159:A:PHE:HB3 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB1 | 2 | 0.18 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB2 | 2 | 0.18 |
| (1,1030) | 1:74:A:PHE:HE1 | 1:162:A:ALA:HB3 | 2 | 0.18 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB1 | 2 | 0.18 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB2 | 2 | 0.18 |
| (1,1030) | 1:74:A:PHE:HE2 | 1:162:A:ALA:HB3 | 2 | 0.18 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 3 | 0.18 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 5 | 0.18 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 7 | 0.18 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 8 | 0.18 |
| (1,922) | 1:70:A:LEU:HD11 | 1:70:A:LEU:H | 7 | 0.18 |
| (1,922) | 1:70:A:LEU:HD12 | 1:70:A:LEU:H | 7 | 0.18 |
| (1,922) | 1:70:A:LEU:HD13 | 1:70:A:LEU:H | 7 | 0.18 |
| (1,914) | 1:69:A:GLN:HG3 | 1:69:A:GLN:H | 8 | 0.18 |
| (1,901) | 1:69:A:GLN:HA | 1:69:A:GLN:HG2 | 4 | 0.18 |
| (1,854) | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3 | 9 | 0.18 |
| (1,849) | 1:66:A:ASN:HD22 | 1:66:A:ASN:H | 4 | 0.18 |
| (1,849) | 1:66:A:ASN:HD22 | 1:66:A:ASN:H | 5 | 0.18 |
| (1,849) | 1:66:A:ASN:HD22 | 1:66:A:ASN:H | 8 | 0.18 |
| (1,845) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA | 4 | 0.18 |
| (1,845) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA | 5 | 0.18 |
| (1,845) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA | 8 | 0.18 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 3 | 0.18 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 4 | 0.18 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 4 | 0.18 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 4 | 0.18 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 4 | 0.18 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 4 | 0.18 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 4 | 0.18 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 4 | 0.18 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 3 | 0.18 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 9 | 0.18 |
| (1,554) | 1:50:A:TRP:HD1 | 1:50:A:TRP:H | 4 | 0.18 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 2 | 0.18 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 9 | 0.18 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG21 | 6 | 0.18 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG22 | 6 | 0.18 |
| (1,545) | 1:50:A:TRP:HA | 1:151:A:VAL:HG23 | 6 | 0.18 |
| (1,541) | 1:50:A:TRP:HA | 1:51:A:ILE:HB | 6 | 0.18 |
| (1,498) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HZ2 | 10 | 0.18 |
| (1,498) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HZ2 | 10 | 0.18 |
| (1,498) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HZ2 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,287) | 1:36:A:ALA:HB1 | 1:36:A:ALA:H | 10 | 0.18 |
| (1,287) | 1:36:A:ALA:HB2 | 1:36:A:ALA:H | 10 | 0.18 |
| (1,287) | 1:36:A:ALA:HB3 | 1:36:A:ALA:H | 10 | 0.18 |
| (1,256) | 1:33:A:THR:HA | 1:168:A:PHE:HZ | 2 | 0.18 |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H | 8 | 0.18 |
| (1,235) | 1:32:A:ILE:HG22 | 1:33:A:THR:H | 8 | 0.18 |
| (1,235) | 1:32:A:ILE:HG23 | 1:33:A:THR:H | 8 | 0.18 |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H | 9 | 0.18 |
| (1,235) | 1:32:A:ILE:HG22 | 1:33:A:THR:H | 9 | 0.18 |
| (1,235) | 1:32:A:ILE:HG23 | 1:33:A:THR:H | 9 | 0.18 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD11 | 5 | 0.18 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD12 | 5 | 0.18 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD13 | 5 | 0.18 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 3 | 0.18 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 4 | 0.18 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 5 | 0.18 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 8 | 0.18 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 6 | 0.18 |
| (1,48) | 1:24:A:ASP:HB3 | 1:50:A:TRP:HD1 | 6 | 0.18 |
| (1,48) | 1:24:A:ASP:HB3 | 1:50:A:TRP:HD1 | 10 | 0.18 |
| (1,46) | 1:24:A:ASP:HB3 | 1:50:A:TRP:HB3 | 6 | 0.18 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 6 | 0.17 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 10 | 0.17 |
| (2,721) | 1:144:A:VAL:HA | 1:145:A:TYR:HD1 | 5 | 0.17 |
| (2,721) | 1:144:A:VAL:HA | 1:145:A:TYR:HD2 | 5 | 0.17 |
| (2,714) | 1:141:A:LYS:HD2 | 1:142:A:ILE:H | 8 | 0.17 |
| (2,714) | 1:141:A:LYS:HD3 | 1:142:A:ILE:H | 8 | 0.17 |
| (2,618) | 1:119:A:ALA:HB1 | 1:149:A:LYS:H | 10 | 0.17 |
| (2,618) | 1:119:A:ALA:HB2 | 1:149:A:LYS:H | 10 | 0.17 |
| (2,618) | 1:119:A:ALA:HB3 | 1:149:A:LYS:H | 10 | 0.17 |
| (2,534) | 1:85:A:TYR:HE1 | 1:151:A:VAL:H | 6 | 0.17 |
| (2,534) | 1:85:A:TYR:HE2 | 1:151:A:VAL:H | 6 | 0.17 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG21 | 7 | 0.17 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG22 | 7 | 0.17 |
| (2,481) | 1:80:A:GLN:HE22 | 1:98:A:THR:HG23 | 7 | 0.17 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE1 | 4 | 0.17 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE2 | 4 | 0.17 |
| (2,339) | 1:59:A:LYS:HE2 | 1:111:A:ILE:H | 10 | 0.17 |
| (2,339) | 1:59:A:LYS:HE3 | 1:111:A:ILE:H | 10 | 0.17 |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H | 3 | 0.17 |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H | 3 | 0.17 |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2455) | 1:182:A:VAL:HA | 1:182:A:VAL:HB | 1 | 0.17 |
| (1,2455) | 1:182:A:VAL:HA | 1:182:A:VAL:HB | 6 | 0.17 |
| (1,2455) | 1:182:A:VAL:HA | 1:182:A:VAL:HB | 8 | 0.17 |
| (1,2455) | 1:182:A:VAL:HA | 1:182:A:VAL:HB | 9 | 0.17 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 7 | 0.17 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 7 | 0.17 |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 7 | 0.17 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 4 | 0.17 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 10 | 0.17 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG21 | 9 | 0.17 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG22 | 9 | 0.17 |
| (1,2347) | 1:173:A:VAL:HB | 1:173:A:VAL:HG23 | 9 | 0.17 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG11 | 9 | 0.17 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG12 | 9 | 0.17 |
| (1,2346) | 1:173:A:VAL:HB | 1:173:A:VAL:HG13 | 9 | 0.17 |
| (1,2316) | 1:171:A:LEU:HA | 1:172:A:PRO:HD3 | 3 | 0.17 |
| (1,2276) | 1:167:A:LEU:H | 1:168:A:PHE:H | 2 | 0.17 |
| (1,2272) | 1:166:A:MET:HB2 | 1:167:A:LEU:H | 1 | 0.17 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 9 | 0.17 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 3 | 0.17 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 8 | 0.17 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 10 | 0.17 |
| (1,2176) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HE1 | 8 | 0.17 |
| (1,2176) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HE2 | 8 | 0.17 |
| (1,2176) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HE1 | 8 | 0.17 |
| (1,2176) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HE2 | 8 | 0.17 |
| (1,1984) | 1:139:A:PRO:HD3 | 1:141:A:LYS:H | 7 | 0.17 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 4 | 0.17 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 6 | 0.17 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 8 | 0.17 |
| (1,1882) | 1:134:A:TRP:HA | 1:143:A:ILE:HA | 5 | 0.17 |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H | 6 | 0.17 |
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H | 6 | 0.17 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 9 | 0.17 |
| (1,1572) | 1:104:A:LEU:HD11 | 1:104:A:LEU:H | 8 | 0.17 |
| (1,1572) | 1:104:A:LEU:HD12 | 1:104:A:LEU:H | 8 | 0.17 |
| (1,1572) | 1:104:A:LEU:HD13 | 1:104:A:LEU:H | 8 | 0.17 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD11 | 1 | 0.17 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD12 | 1 | 0.17 |
| (1,1522) | 1:100:A:ALA:H | 1:111:A:ILE:HD13 | 1 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 2 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 2 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 2 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 4 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 4 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 4 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 7 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 7 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 7 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 8 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 8 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 8 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 10 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 10 | 0.17 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 10 | 0.17 |
| (1,1371) | 1:86:A:GLU:H | 1:134:A:TRP:HE1 | 9 | 0.17 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG21 | 1 | 0.17 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG22 | 1 | 0.17 |
| (1,1342) | 1:85:A:TYR:HE1 | 1:143:A:ILE:HG23 | 1 | 0.17 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG21 | 1 | 0.17 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG22 | 1 | 0.17 |
| (1,1342) | 1:85:A:TYR:HE2 | 1:143:A:ILE:HG23 | 1 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 2 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 2 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 2 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 4 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 4 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 4 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 9 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 9 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 9 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 10 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 10 | 0.17 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 10 | 0.17 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 2 | 0.17 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 10 | 0.17 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 10 | 0.17 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 10 | 0.17 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 10 | 0.17 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 10 | 0.17 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 10 | 0.17 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 6 | 0.17 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 6 | 0.17 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 6 | 0.17 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 6 | 0.17 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 6 | 0.17 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 6 | 0.17 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 6 | 0.17 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 6 | 0.17 |
| (1,1128) | 1:78:A:GLN:H | 1:158:A:ALA:HA | 4 | 0.17 |
| (1,1116) | 1:78:A:GLN:HB3 | 1:78:A:GLN:H | 1 | 0.17 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 1 | 0.17 |
| (1,911) | 1:69:A:GLN:HE22 | 1:70:A:LEU:H | 3 | 0.17 |
| (1,911) | 1:69:A:GLN:HE22 | 1:70:A:LEU:H | 4 | 0.17 |
| (1,908) | 1:69:A:GLN:HB3 | 1:70:A:LEU:H | 2 | 0.17 |
| (1,857) | 1:66:A:ASN:HD22 | 1:174:A:ILE:H | 8 | 0.17 |
| (1,849) | 1:66:A:ASN:HD22 | 1:66:A:ASN:H | 3 | 0.17 |
| (1,837) | 1:66:A:ASN:HB2 | 1:66:A:ASN:HD22 | 10 | 0.17 |
| (1,829) | 1:66:A:ASN:HA | 1:69:A:GLN:HG2 | 4 | 0.17 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 2 | 0.17 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 2 | 0.17 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 2 | 0.17 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 2 | 0.17 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 2 | 0.17 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 2 | 0.17 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 2 | 0.17 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 2 | 0.17 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 2 | 0.17 |
| (1,761) | 1:63:A:THR:H | 1:175:A:PHE:HA | 6 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 1 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 1 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 1 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 2 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 2 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 2 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 3 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 3 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 3 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 5 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 5 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 5 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 6 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 6 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 6 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 7 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 7 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 8 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 8 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 8 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG21 | 9 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG22 | 9 | 0.17 |
| (1,745) | 1:63:A:THR:HB | 1:63:A:THR:HG23 | 9 | 0.17 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 7 | 0.17 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 7 | 0.17 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 7 | 0.17 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 10 | 0.17 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 10 | 0.17 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 10 | 0.17 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 1 | 0.17 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 2 | 0.17 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 3 | 0.17 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 9 | 0.17 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD11 | 7 | 0.17 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD12 | 7 | 0.17 |
| (1,655) | 1:58:A:VAL:H | 1:113:A:LEU:HD13 | 7 | 0.17 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 3 | 0.17 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 3 | 0.17 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 3 | 0.17 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 3 | 0.17 |
| (1,541) | 1:50:A:TRP:HA | 1:51:A:ILE:HB | 4 | 0.17 |
| (1,541) | 1:50:A:TRP:HA | 1:51:A:ILE:HB | 7 | 0.17 |
| (1,530) | 1:49:A:VAL:H | 1:152:A:ALA:HA | 6 | 0.17 |
| (1,530) | 1:49:A:VAL:H | 1:152:A:ALA:HA | 10 | 0.17 |
| (1,496) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HH2 | 6 | 0.17 |
| (1,496) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HH2 | 6 | 0.17 |
| (1,496) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HH2 | 6 | 0.17 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG21 | 9 | 0.17 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG22 | 9 | 0.17 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG23 | 9 | 0.17 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE1 | 3 | 0.17 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE2 | 3 | 0.17 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 7 | 0.17 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 7 | 0.17 |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 7 | 0.17 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 7 | 0.17 |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 7 | 0.17 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 7 | 0.17 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 7 | 0.17 |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 7 | 0.17 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 5 | 0.17 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD11 | 8 | 0.17 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD12 | 8 | 0.17 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD13 | 8 | 0.17 |
| (1,166) | 1:29:A:LEU:HD11 | 1:175:A:PHE:H | 4 | 0.17 |
| (1,166) | 1:29:A:LEU:HD12 | 1:175:A:PHE:H | 4 | 0.17 |
| (1,166) | 1:29:A:LEU:HD13 | 1:175:A:PHE:H | 4 | 0.17 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 2 | 0.17 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 10 | 0.17 |
| (1,46) | 1:24:A:ASP:HB3 | 1:50:A:TRP:HB3 | 10 | 0.17 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG21 | 3 | 0.17 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG22 | 3 | 0.17 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG23 | 3 | 0.17 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 3 | 0.16 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD11 | 9 | 0.16 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD12 | 9 | 0.16 |
| (2,765) | 1:169:A:ASP:H | 1:171:A:LEU:HD13 | 9 | 0.16 |
| (2,761) | 1:168:A:PHE:H | 1:169:A:ASP:H | 10 | 0.16 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD21 | 4 | 0.16 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD22 | 4 | 0.16 |
| (2,756) | 1:167:A:LEU:H | 1:167:A:LEU:HD23 | 4 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 3 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 3 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 3 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 5 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 5 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 5 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 6 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 6 | 0.16 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 6 | 0.16 |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H | 4 | 0.16 |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H | 4 | 0.16 |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H | 4 | 0.16 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 3 | 0.16 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 3 | 0.16 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 3 | 0.16 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 5 | 0.16 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 5 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 5 | 0.16 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 6 | 0.16 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 6 | 0.16 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 6 | 0.16 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD1 | 5 | 0.16 |
| (2,733) | 1:157:A:LYS:HE2 | 1:159:A:PHE:HD2 | 5 | 0.16 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD1 | 5 | 0.16 |
| (2,733) | 1:157:A:LYS:HE3 | 1:159:A:PHE:HD2 | 5 | 0.16 |
| (1,2316) | 1:171:A:LEU:HA | 1:172:A:PRO:HD3 | 10 | 0.16 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD21 | 2 | 0.16 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD22 | 2 | 0.16 |
| (1,2304) | 1:170:A:SER:HA | 1:171:A:LEU:HD23 | 2 | 0.16 |
| (1,2287) | 1:168:A:PHE:HD1 | 1:169:A:ASP:H | 1 | 0.16 |
| (1,2287) | 1:168:A:PHE:HD2 | 1:169:A:ASP:H | 1 | 0.16 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 3 | 0.16 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 5 | 0.16 |
| (1,2260) | 1:163:A:LYS:H | 1:168:A:PHE:HZ | 6 | 0.16 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 4 | 0.16 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 5 | 0.16 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 7 | 0.16 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 2 | 0.16 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 7 | 0.16 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 9 | 0.16 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 10 | 0.16 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 10 | 0.16 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 10 | 0.16 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 10 | 0.16 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 10 | 0.16 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 10 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 3 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 3 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 3 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 4 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 4 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 4 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 5 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 5 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 5 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 9 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 9 | 0.16 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 9 | 0.16 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1774) | 1:121:A:LEU:HB3 | 1:121:A:LEU:H | 10 | 0.16 |
| (1,1648) | 1:112:A:VAL:HG21 | 1:112:A:VAL:H | 6 | 0.16 |
| (1,1648) | 1:112:A:VAL:HG22 | 1:112:A:VAL:H | 6 | 0.16 |
| (1,1648) | 1:112:A:VAL:HG23 | 1:112:A:VAL:H | 6 | 0.16 |
| (1,1603) | 1:107:A:PRO:HB3 | 1:108:A:SER:HA | 7 | 0.16 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 5 | 0.16 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 6 | 0.16 |
| (1,1505) | 1:98:A:THR:HA | 1:100:A:ALA:H | 4 | 0.16 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 7 | 0.16 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG21 | 5 | 0.16 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG22 | 5 | 0.16 |
| (1,1383) | 1:87:A:THR:HB | 1:87:A:THR:HG23 | 5 | 0.16 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG21 | 10 | 0.16 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG22 | 10 | 0.16 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG23 | 10 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 1 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 1 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 1 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 3 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 3 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 3 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 5 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 5 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 5 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 6 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 6 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 6 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 7 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 7 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 7 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG21 | 8 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG22 | 8 | 0.16 |
| (1,1261) | 1:82:A:THR:HB | 1:82:A:THR:HG23 | 8 | 0.16 |
| (1,1232) | 1:81:A:ILE:HG21 | 1:99:A:LYS:H | 1 | 0.16 |
| (1,1232) | 1:81:A:ILE:HG22 | 1:99:A:LYS:H | 1 | 0.16 |
| (1,1232) | 1:81:A:ILE:HG23 | 1:99:A:LYS:H | 1 | 0.16 |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H | 6 | 0.16 |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H | 6 | 0.16 |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H | 6 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 4 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 4 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 4 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 4 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 4 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 4 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 4 | 0.16 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 4 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 8 | 0.16 |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 8 | 0.16 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 5 | 0.16 |
| (1,922) | 1:70:A:LEU:HD11 | 1:70:A:LEU:H | 9 | 0.16 |
| (1,922) | 1:70:A:LEU:HD12 | 1:70:A:LEU:H | 9 | 0.16 |
| (1,922) | 1:70:A:LEU:HD13 | 1:70:A:LEU:H | 9 | 0.16 |
| (1,914) | 1:69:A:GLN:HG3 | 1:69:A:GLN:H | 3 | 0.16 |
| (1,914) | 1:69:A:GLN:HG3 | 1:69:A:GLN:H | 5 | 0.16 |
| (1,908) | 1:69:A:GLN:HB3 | 1:70:A:LEU:H | 6 | 0.16 |
| (1,857) | 1:66:A:ASN:HD22 | 1:174:A:ILE:H | 1 | 0.16 |
| (1,857) | 1:66:A:ASN:HD22 | 1:174:A:ILE:H | 2 | 0.16 |
| (1,845) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA | 3 | 0.16 |
| (1,845) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA | 10 | 0.16 |
| (1,762) | 1:63:A:THR:H | 1:175:A:PHE:HD1 | 6 | 0.16 |
| (1,762) | 1:63:A:THR:H | 1:175:A:PHE:HD2 | 6 | 0.16 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 1 | 0.16 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 1 | 0.16 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 1 | 0.16 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 2 | 0.16 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 2 | 0.16 |
| (1,684) | 1:60:A:LEU:H | 1:61:A:LYS:H | 10 | 0.16 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 1 | 0.16 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 2 | 0.16 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 4 | 0.16 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 6 | 0.16 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 7 | 0.16 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 10 | 0.16 |
| (1,627) | 1:56:A:ASN:HB2 | 1:56:A:ASN:HD21 | 6 | 0.16 |
| (1,627) | 1:56:A:ASN:HB3 | 1:56:A:ASN:HD21 | 6 | 0.16 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 5 | 0.16 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 9 | 0.16 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 9 | 0.16 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 9 | 0.16 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 10 | 0.16 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 10 | 0.16 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 10 | 0.16 |
| (1,554) | 1:50:A:TRP:HD1 | 1:50:A:TRP:H | 2 | 0.16 |
| (1,554) | 1:50:A:TRP:HD1 | 1:50:A:TRP:H | 8 | 0.16 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG21 | 5 | 0.16 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG22 | 5 | 0.16 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG23 | 5 | 0.16 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG21 | 10 | 0.16 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG22 | 10 | 0.16 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG23 | 10 | 0.16 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE1 | 8 | 0.16 |
| (1,467) | 1:47:A:ALA:H | 1:156:A:PHE:HE2 | 8 | 0.16 |
| (1,455) | 1:47:A:ALA:HB1 | 1:48:A:ILE:H | 5 | 0.16 |
| (1,455) | 1:47:A:ALA:HB2 | 1:48:A:ILE:H | 5 | 0.16 |
| (1,455) | 1:47:A:ALA:HB3 | 1:48:A:ILE:H | 5 | 0.16 |
| (1,455) | 1:47:A:ALA:HB1 | 1:48:A:ILE:H | 8 | 0.16 |
| (1,455) | 1:47:A:ALA:HB2 | 1:48:A:ILE:H | 8 | 0.16 |
| (1,455) | 1:47:A:ALA:HB3 | 1:48:A:ILE:H | 8 | 0.16 |
| (1,426) | 1:46:A:TYR:HA | 1:156:A:PHE:HA | 4 | 0.16 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 3 | 0.16 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 3 | 0.16 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 3 | 0.16 |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H | 9 | 0.16 |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H | 9 | 0.16 |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H | 9 | 0.16 |
| (1,339) | 1:41:A:SER:HB2 | 1:159:A:PHE:HD1 | 5 | 0.16 |
| (1,339) | 1:41:A:SER:HB2 | 1:159:A:PHE:HD2 | 5 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,295) | 1:38:A:ALA:HA | 1:39:A:GLN:H | 10 | 0.16 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 5 | 0.16 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 4 | 0.16 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 4 | 0.16 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 4 | 0.16 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 2 | 0.16 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 9 | 0.16 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 1 | 0.16 |
| (3,13) | 1:181:A:GLN:HA | 1:181:A:GLN:HB2 | 7 | 0.15 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 1 | 0.15 |
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 8 | 0.15 |
| (3,2) | 1:33:A:THR:HA | 1:34:A:PRO:HD3 | 4 | 0.15 |
| (2,770) | 1:174:A:ILE:HG21 | 1:176:A:ASN:HA | 8 | 0.15 |
| (2,770) | 1:174:A:ILE:HG22 | 1:176:A:ASN:HA | 8 | 0.15 |
| (2,770) | 1:174:A:ILE:HG23 | 1:176:A:ASN:HA | 8 | 0.15 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD11 | 9 | 0.15 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD12 | 9 | 0.15 |
| (2,755) | 1:167:A:LEU:H | 1:167:A:LEU:HD13 | 9 | 0.15 |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H | 9 | 0.15 |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H | 9 | 0.15 |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H | 9 | 0.15 |
| (2,744) | 1:163:A:LYS:HG3 | 1:166:A:MET:H | 9 | 0.15 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 5 | 0.15 |
| (2,534) | 1:85:A:TYR:HE1 | 1:151:A:VAL:H | 4 | 0.15 |
| (2,534) | 1:85:A:TYR:HE2 | 1:151:A:VAL:H | 4 | 0.15 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 2 | 0.15 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 2 | 0.15 |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 2 | 0.15 |
| (1,2349) | 1:173:A:VAL:HB | 1:174:A:ILE:H | 3 | 0.15 |
| (1,2299) | 1:169:A:ASP:H | 1:170:A:SER:H | 8 | 0.15 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 4 | 0.15 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 7 | 0.15 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 8 | 0.15 |
| (1,2258) | 1:163:A:LYS:HG2 | 1:163:A:LYS:H | 10 | 0.15 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 6 | 0.15 |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H | 7 | 0.15 |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H | 7 | 0.15 |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H | 7 | 0.15 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 4 | 0.15 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 5 | 0.15 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG21 | 5 | 0.15 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG22 | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG23 | 5 | 0.15 |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H | 4 | 0.15 |
| (1,1778) | 1:121:A:LEU:HG | 1:121:A:LEU:H | 1 | 0.15 |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H | 5 | 0.15 |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H | 5 | 0.15 |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H | 5 | 0.15 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 6 | 0.15 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 7 | 0.15 |
| (1,1639) | 1:111:A:ILE:HG21 | 1:111:A:ILE:H | 8 | 0.15 |
| (1,1639) | 1:111:A:ILE:HG22 | 1:111:A:ILE:H | 8 | 0.15 |
| (1,1639) | 1:111:A:ILE:HG23 | 1:111:A:ILE:H | 8 | 0.15 |
| (1,1572) | 1:104:A:LEU:HD11 | 1:104:A:LEU:H | 7 | 0.15 |
| (1,1572) | 1:104:A:LEU:HD12 | 1:104:A:LEU:H | 7 | 0.15 |
| (1,1572) | 1:104:A:LEU:HD13 | 1:104:A:LEU:H | 7 | 0.15 |
| (1,1534) | 1:102:A:ILE:HB | 1:103:A:SER:H | 4 | 0.15 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 3 | 0.15 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 3 | 0.15 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 3 | 0.15 |
| (1,1505) | 1:98:A:THR:HA | 1:100:A:ALA:H | 8 | 0.15 |
| (1,1460) | 1:92:A:LEU:HG | 1:93:A:GLY:H | 4 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 1 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 2 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 3 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 4 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 5 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 6 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 8 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 9 | 0.15 |
| (1,1425) | 1:88:A:ASN:HD21 | 1:88:A:ASN:HD22 | 10 | 0.15 |
| (1,1402) | 1:87:A:THR:HG21 | 1:89:A:SER:H | 2 | 0.15 |
| (1,1402) | 1:87:A:THR:HG22 | 1:89:A:SER:H | 2 | 0.15 |
| (1,1402) | 1:87:A:THR:HG23 | 1:89:A:SER:H | 2 | 0.15 |
| (1,1363) | 1:86:A:GLU:HG3 | 1:86:A:GLU:H | 1 | 0.15 |
| (1,1363) | 1:86:A:GLU:HG3 | 1:86:A:GLU:H | 8 | 0.15 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 6 | 0.15 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 6 | 0.15 |
| (1,1338) | 1:85:A:TYR:HD1 | 1:86:A:GLU:H | 7 | 0.15 |
| (1,1338) | 1:85:A:TYR:HD2 | 1:86:A:GLU:H | 7 | 0.15 |
| (1,1314) | 1:83:A:SER:H | 1:99:A:LYS:HE2 | 4 | 0.15 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB1 | 1 | 0.15 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB2 | 1 | 0.15 |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB3 | 1 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB1 | 1 | 0.15 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB2 | 1 | 0.15 |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB3 | 1 | 0.15 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB1 | 1 | 0.15 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB2 | 1 | 0.15 |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB3 | 1 | 0.15 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 2 | 0.15 |
| (1,1128) | 1:78:A:GLN:H | 1:158:A:ALA:HA | 3 | 0.15 |
| (1,1128) | 1:78:A:GLN:H | 1:158:A:ALA:HA | 7 | 0.15 |
| (1,1127) | 1:78:A:GLN:H | 1:104:A:LEU:H | 9 | 0.15 |
| (1,1100) | 1:77:A:LEU:HG | 1:78:A:GLN:H | 4 | 0.15 |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3 | 4 | 0.15 |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3 | 4 | 0.15 |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3 | 4 | 0.15 |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3 | 4 | 0.15 |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3 | 4 | 0.15 |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3 | 4 | 0.15 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 1 | 0.15 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 4 | 0.15 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 10 | 0.15 |
| (1,989) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HE1 | 3 | 0.15 |
| (1,989) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HE2 | 3 | 0.15 |
| (1,989) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HE1 | 3 | 0.15 |
| (1,989) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HE2 | 3 | 0.15 |
| (1,922) | 1:70:A:LEU:HD11 | 1:70:A:LEU:H | 1 | 0.15 |
| (1,922) | 1:70:A:LEU:HD12 | 1:70:A:LEU:H | 1 | 0.15 |
| (1,922) | 1:70:A:LEU:HD13 | 1:70:A:LEU:H | 1 | 0.15 |
| (1,912) | 1:69:A:GLN:HG3 | 1:69:A:GLN:HE21 | 10 | 0.15 |
| (1,909) | 1:69:A:GLN:HB2 | 1:70:A:LEU:H | 8 | 0.15 |
| (1,899) | 1:69:A:GLN:HA | 1:69:A:GLN:HE22 | 9 | 0.15 |
| (1,894) | 1:68:A:GLU:H | 1:69:A:GLN:H | 3 | 0.15 |
| (1,894) | 1:68:A:GLU:H | 1:69:A:GLN:H | 5 | 0.15 |
| (1,856) | 1:66:A:ASN:HD22 | 1:173:A:VAL:HA | 9 | 0.15 |
| (1,854) | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3 | 10 | 0.15 |
| (1,831) | 1:66:A:ASN:HA | 1:174:A:ILE:HB | 3 | 0.15 |
| (1,831) | 1:66:A:ASN:HA | 1:174:A:ILE:HB | 8 | 0.15 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 9 | 0.15 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 9 | 0.15 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 9 | 0.15 |
| (1,651) | 1:58:A:VAL:HG11 | 1:59:A:LYS:H | 7 | 0.15 |
| (1,651) | 1:58:A:VAL:HG12 | 1:59:A:LYS:H | 7 | 0.15 |
| (1,651) | 1:58:A:VAL:HG13 | 1:59:A:LYS:H | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,651) | 1:58:A:VAL:HG21 | 1:59:A:LYS:H | 7 | 0.15 |
| (1,651) | 1:58:A:VAL:HG22 | 1:59:A:LYS:H | 7 | 0.15 |
| (1,651) | 1:58:A:VAL:HG23 | 1:59:A:LYS:H | 7 | 0.15 |
| (1,633) | 1:56:A:ASN:HD22 | 1:57:A:ASP:H | 6 | 0.15 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 3 | 0.15 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 5 | 0.15 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 8 | 0.15 |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 9 | 0.15 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 2 | 0.15 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 8 | 0.15 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB2 | 3 | 0.15 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB3 | 3 | 0.15 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB2 | 3 | 0.15 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB3 | 3 | 0.15 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB2 | 3 | 0.15 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB3 | 3 | 0.15 |
| (1,573) | 1:51:A:ILE:HD11 | 1:55:A:VAL:H | 10 | 0.15 |
| (1,573) | 1:51:A:ILE:HD12 | 1:55:A:VAL:H | 10 | 0.15 |
| (1,573) | 1:51:A:ILE:HD13 | 1:55:A:VAL:H | 10 | 0.15 |
| (1,561) | 1:50:A:TRP:HE3 | 1:151:A:VAL:HG21 | 6 | 0.15 |
| (1,561) | 1:50:A:TRP:HE3 | 1:151:A:VAL:HG22 | 6 | 0.15 |
| (1,561) | 1:50:A:TRP:HE3 | 1:151:A:VAL:HG23 | 6 | 0.15 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 7 | 0.15 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 10 | 0.15 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 10 | 0.15 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 10 | 0.15 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG21 | 6 | 0.15 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG22 | 6 | 0.15 |
| (1,470) | 1:48:A:ILE:HA | 1:48:A:ILE:HG23 | 6 | 0.15 |
| (1,292) | 1:37:A:GLY:HA2 | 1:37:A:GLY:H | 8 | 0.15 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 10 | 0.15 |
| (1,241) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HD1 | 1 | 0.15 |
| (1,241) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HD2 | 1 | 0.15 |
| (1,241) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HD1 | 1 | 0.15 |
| (1,241) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HD2 | 1 | 0.15 |
| (1,241) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HD1 | 1 | 0.15 |
| (1,241) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HD2 | 1 | 0.15 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 8 | 0.15 |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H | 1 | 0.15 |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H | 9 | 0.15 |
| (1,208) | 1:32:A:ILE:HA | 1:32:A:ILE:HG12 | 10 | 0.15 |
| (1,100) | 1:26:A:GLU:HB2 | 1:50:A:TRP:HE1 | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,54) | 1:24:A:ASP:HB2 | 1:50:A:TRP:HB2 | 6 | 0.15 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 3 | 0.15 |
| (3,12) | 1:181:A:GLN:HA | 1:181:A:GLN:HB3 | 5 | 0.14 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 7 | 0.14 |
| (2,628) | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2 | 10 | 0.14 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG2 | 4 | 0.14 |
| (2,607) | 1:115:A:LYS:H | 1:116:A:GLU:HG3 | 4 | 0.14 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 2 | 0.14 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 2 | 0.14 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 2 | 0.14 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 2 | 0.14 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD1 | 1 | 0.14 |
| (2,517) | 1:84:A:GLY:HA2 | 1:85:A:TYR:HD2 | 1 | 0.14 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD1 | 1 | 0.14 |
| (2,517) | 1:84:A:GLY:HA3 | 1:85:A:TYR:HD2 | 1 | 0.14 |
| (2,510) | 1:83:A:SER:HB3 | 1:154:A:LEU:HA | 2 | 0.14 |
| (2,298) | 1:54:A:GLN:HB3 | 1:54:A:GLN:HE21 | 8 | 0.14 |
| (2,206) | 1:39:A:GLN:HB2 | 1:39:A:GLN:HE21 | 1 | 0.14 |
| (2,206) | 1:39:A:GLN:HB2 | 1:39:A:GLN:HE21 | 6 | 0.14 |
| (2,206) | 1:39:A:GLN:HB2 | 1:39:A:GLN:HE21 | 7 | 0.14 |
| (2,205) | 1:39:A:GLN:HB3 | 1:39:A:GLN:HE21 | 3 | 0.14 |
| (2,205) | 1:39:A:GLN:HB3 | 1:39:A:GLN:HE21 | 4 | 0.14 |
| (2,205) | 1:39:A:GLN:HB3 | 1:39:A:GLN:HE21 | 5 | 0.14 |
| (2,205) | 1:39:A:GLN:HB3 | 1:39:A:GLN:HE21 | 8 | 0.14 |
| (2,205) | 1:39:A:GLN:HB3 | 1:39:A:GLN:HE21 | 9 | 0.14 |
| (2,178) | 1:36:A:ALA:H | 1:37:A:GLY:H | 2 | 0.14 |
| (2,12) | 1:17:A:GLN:HB2 | 1:17:A:GLN:HE21 | 5 | 0.14 |
| (2,12) | 1:17:A:GLN:HB2 | 1:17:A:GLN:HE21 | 7 | 0.14 |
| (2,11) | 1:17:A:GLN:HB3 | 1:17:A:GLN:HE21 | 8 | 0.14 |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H | 4 | 0.14 |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H | 4 | 0.14 |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H | 4 | 0.14 |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA | 1 | 0.14 |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA | 1 | 0.14 |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA | 1 | 0.14 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 8 | 0.14 |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 8 | 0.14 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 8 | 0.14 |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 8 | 0.14 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 8 | 0.14 |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 8 | 0.14 |
| (1,2342) | 1:173:A:VAL:HA | 1:173:A:VAL:HG11 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2342) | 1:173:A:VAL:HA | 1:173:A:VAL:HG12 | 6 | 0.14 |
| (1,2342) | 1:173:A:VAL:HA | 1:173:A:VAL:HG13 | 6 | 0.14 |
| (1,2299) | 1:169:A:ASP:H | 1:170:A:SER:H | 10 | 0.14 |
| (1,2283) | 1:168:A:PHE:HB2 | 1:168:A:PHE:H | 2 | 0.14 |
| (1,2260) | 1:163:A:LYS:H | 1:168:A:PHE:HZ | 2 | 0.14 |
| (1,2258) | 1:163:A:LYS:HG2 | 1:163:A:LYS:H | 5 | 0.14 |
| (1,2258) | 1:163:A:LYS:HG2 | 1:163:A:LYS:H | 8 | 0.14 |
| (1,2190) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HD1 | 2 | 0.14 |
| (1,2190) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HD2 | 2 | 0.14 |
| (1,2190) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HD1 | 2 | 0.14 |
| (1,2190) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HD2 | 2 | 0.14 |
| (1,2190) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HD1 | 2 | 0.14 |
| (1,2190) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HD2 | 2 | 0.14 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 5 | 0.14 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 6 | 0.14 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 6 | 0.14 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 6 | 0.14 |
| (1,2069) | 1:148:A:THR:HG21 | 1:148:A:THR:H | 5 | 0.14 |
| (1,2069) | 1:148:A:THR:HG22 | 1:148:A:THR:H | 5 | 0.14 |
| (1,2069) | 1:148:A:THR:HG23 | 1:148:A:THR:H | 5 | 0.14 |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H | 6 | 0.14 |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H | 6 | 0.14 |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H | 6 | 0.14 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 7 | 0.14 |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H | 1 | 0.14 |
| (1,1847) | 1:132:A:SER:H | 1:134:A:TRP:HH2 | 8 | 0.14 |
| (1,1834) | 1:132:A:SER:HA | 1:145:A:TYR:HB3 | 5 | 0.14 |
| (1,1793) | 1:128:A:TYR:HA | 1:128:A:TYR:HB3 | 6 | 0.14 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG21 | 3 | 0.14 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG22 | 3 | 0.14 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG23 | 3 | 0.14 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG21 | 7 | 0.14 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG22 | 7 | 0.14 |
| (1,1790) | 1:126:A:THR:HA | 1:126:A:THR:HG23 | 7 | 0.14 |
| (1,1775) | 1:121:A:LEU:HB2 | 1:121:A:LEU:H | 8 | 0.14 |
| (1,1774) | 1:121:A:LEU:HB3 | 1:121:A:LEU:H | 5 | 0.14 |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H | 5 | 0.14 |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H | 5 | 0.14 |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H | 5 | 0.14 |
| (1,1510) | 1:98:A:THR:HG21 | 1:100:A:ALA:H | 6 | 0.14 |
| (1,1510) | 1:98:A:THR:HG22 | 1:100:A:ALA:H | 6 | 0.14 |
| (1,1510) | 1:98:A:THR:HG23 | 1:100:A:ALA:H | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1443) | 1:89:A:SER:H | 1:134:A:TRP:HH2 | 5 | 0.14 |
| (1,1419) | 1:88:A:ASN:HB3 | 1:88:A:ASN:HD21 | 5 | 0.14 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 4 | 0.14 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 4 | 0.14 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 4 | 0.14 |
| (1,1380) | 1:87:A:THR:HA | 1:134:A:TRP:HH2 | 2 | 0.14 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 10 | 0.14 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 10 | 0.14 |
| (1,1335) | 1:85:A:TYR:HB2 | 1:86:A:GLU:H | 2 | 0.14 |
| (1,1335) | 1:85:A:TYR:HB2 | 1:86:A:GLU:H | 4 | 0.14 |
| (1,1273) | 1:82:A:THR:HG21 | 1:96:A:SER:HA | 7 | 0.14 |
| (1,1273) | 1:82:A:THR:HG22 | 1:96:A:SER:HA | 7 | 0.14 |
| (1,1273) | 1:82:A:THR:HG23 | 1:96:A:SER:HA | 7 | 0.14 |
| (1,1273) | 1:82:A:THR:HG21 | 1:96:A:SER:HA | 8 | 0.14 |
| (1,1273) | 1:82:A:THR:HG22 | 1:96:A:SER:HA | 8 | 0.14 |
| (1,1273) | 1:82:A:THR:HG23 | 1:96:A:SER:HA | 8 | 0.14 |
| (1,1272) | 1:82:A:THR:HG21 | 1:96:A:SER:HA | 7 | 0.14 |
| (1,1272) | 1:82:A:THR:HG22 | 1:96:A:SER:HA | 7 | 0.14 |
| (1,1272) | 1:82:A:THR:HG23 | 1:96:A:SER:HA | 7 | 0.14 |
| (1,1272) | 1:82:A:THR:HG21 | 1:96:A:SER:HA | 8 | 0.14 |
| (1,1272) | 1:82:A:THR:HG22 | 1:96:A:SER:HA | 8 | 0.14 |
| (1,1272) | 1:82:A:THR:HG23 | 1:96:A:SER:HA | 8 | 0.14 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 3 | 0.14 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 6 | 0.14 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 9 | 0.14 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 3 | 0.14 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 7 | 0.14 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 9 | 0.14 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 1 | 0.14 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 7 | 0.14 |
| (1,926) | 1:70:A:LEU:HD21 | 1:70:A:LEU:H | 4 | 0.14 |
| (1,926) | 1:70:A:LEU:HD22 | 1:70:A:LEU:H | 4 | 0.14 |
| (1,926) | 1:70:A:LEU:HD23 | 1:70:A:LEU:H | 4 | 0.14 |
| (1,909) | 1:69:A:GLN:HB2 | 1:70:A:LEU:H | 2 | 0.14 |
| (1,886) | 1:68:A:GLU:HA | 1:71:A:LYS:HD2 | 10 | 0.14 |
| (1,886) | 1:68:A:GLU:HA | 1:71:A:LYS:HD3 | 10 | 0.14 |
| (1,880) | 1:68:A:GLU:HA | 1:68:A:GLU:HG3 | 6 | 0.14 |
| (1,863) | 1:66:A:ASN:H | 1:175:A:PHE:HA | 1 | 0.14 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 6 | 0.14 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 6 | 0.14 |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 6 | 0.14 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 6 | 0.14 |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 6 | 0.14 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 6 | 0.14 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 6 | 0.14 |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 6 | 0.14 |
| (1,683) | 1:60:A:LEU:HG | 1:60:A:LEU:H | 6 | 0.14 |
| (1,683) | 1:60:A:LEU:HG | 1:60:A:LEU:H | 9 | 0.14 |
| (1,597) | 1:53:A:ASP:HB2 | 1:54:A:GLN:H | 4 | 0.14 |
| (1,597) | 1:53:A:ASP:HB3 | 1:54:A:GLN:H | 4 | 0.14 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB2 | 2 | 0.14 |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB3 | 2 | 0.14 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB2 | 2 | 0.14 |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB3 | 2 | 0.14 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB2 | 2 | 0.14 |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB3 | 2 | 0.14 |
| (1,554) | 1:50:A:TRP:HD1 | 1:50:A:TRP:H | 7 | 0.14 |
| (1,529) | 1:49:A:VAL:H | 1:151:A:VAL:HA | 3 | 0.14 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 6 | 0.14 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 6 | 0.14 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 6 | 0.14 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG21 | 5 | 0.14 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG22 | 5 | 0.14 |
| (1,461) | 1:47:A:ALA:H | 1:153:A:ILE:HG23 | 5 | 0.14 |
| (1,447) | 1:46:A:TYR:HE1 | 1:141:A:LYS:HG3 | 3 | 0.14 |
| (1,447) | 1:46:A:TYR:HE2 | 1:141:A:LYS:HG3 | 3 | 0.14 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG21 | 9 | 0.14 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG22 | 9 | 0.14 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG23 | 9 | 0.14 |
| (1,426) | 1:46:A:TYR:HA | 1:156:A:PHE:HA | 5 | 0.14 |
| (1,337) | 1:41:A:SER:HB2 | 1:42:A:ASP:HA | 5 | 0.14 |
| (1,337) | 1:41:A:SER:HB2 | 1:42:A:ASP:HA | 9 | 0.14 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 6 | 0.14 |
| (1,256) | 1:33:A:THR:HA | 1:168:A:PHE:HZ | 6 | 0.14 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 4 | 0.14 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 9 | 0.14 |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H | 8 | 0.14 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 8 | 0.14 |
| (1,139) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 8 | 0.14 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 10 | 0.14 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 4 | 0.14 |
| (1,12) | 1:21:A:GLU:HA | 1:21:A:GLU:HG2 | 1 | 0.14 |
| (1,12) | 1:21:A:GLU:HA | 1:21:A:GLU:HG3 | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,4) | 1:57:A:ASP:HA | 1:114:A:ASP:HA | 5 | 0.13 |
| (2,761) | 1:168:A:PHE:H | 1:169:A:ASP:H | 2 | 0.13 |
| (2,760) | 1:168:A:PHE:HE1 | 1:171:A:LEU:HG | 6 | 0.13 |
| (2,760) | 1:168:A:PHE:HE2 | 1:171:A:LEU:HG | 6 | 0.13 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD1 | 4 | 0.13 |
| (2,731) | 1:155:A:ASN:H | 1:156:A:PHE:HD2 | 4 | 0.13 |
| (2,625) | 1:121:A:LEU:H | 1:122:A:TYR:HD1 | 8 | 0.13 |
| (2,625) | 1:121:A:LEU:H | 1:122:A:TYR:HD2 | 8 | 0.13 |
| (2,574) | 1:92:A:LEU:H | 1:94:A:ASN:H | 7 | 0.13 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD1 | 2 | 0.13 |
| (2,383) | 1:70:A:LEU:HA | 1:74:A:PHE:HD2 | 2 | 0.13 |
| (2,298) | 1:54:A:GLN:HB3 | 1:54:A:GLN:HE21 | 10 | 0.13 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD11 | 7 | 0.13 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD12 | 7 | 0.13 |
| (1,2313) | 1:171:A:LEU:HA | 1:171:A:LEU:HD13 | 7 | 0.13 |
| (1,2271) | 1:166:A:MET:HB3 | 1:167:A:LEU:H | 6 | 0.13 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 1 | 0.13 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 6 | 0.13 |
| (1,2260) | 1:163:A:LYS:H | 1:168:A:PHE:HZ | 8 | 0.13 |
| (1,2258) | 1:163:A:LYS:HG2 | 1:163:A:LYS:H | 3 | 0.13 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 2 | 0.13 |
| (1,2191) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HE1 | 4 | 0.13 |
| (1,2191) | 1:158:A:ALA:HB1 | 1:160:A:TYR:HE2 | 4 | 0.13 |
| (1,2191) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HE1 | 4 | 0.13 |
| (1,2191) | 1:158:A:ALA:HB2 | 1:160:A:TYR:HE2 | 4 | 0.13 |
| (1,2191) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HE1 | 4 | 0.13 |
| (1,2191) | 1:158:A:ALA:HB3 | 1:160:A:TYR:HE2 | 4 | 0.13 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 3 | 0.13 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 4 | 0.13 |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H | 9 | 0.13 |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H | 9 | 0.13 |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H | 9 | 0.13 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 1 | 0.13 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 1 | 0.13 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 1 | 0.13 |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H | 10 | 0.13 |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H | 10 | 0.13 |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H | 10 | 0.13 |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H | 1 | 0.13 |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H | 1 | 0.13 |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H | 1 | 0.13 |
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD21 | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1953) | 1:136:A:PRO:HG3 | 1:155:A:ASN:HD22 | 2 | 0.13 |
| (1,1880) | 1:134:A:TRP:HA | 1:142:A:ILE:HG21 | 5 | 0.13 |
| (1,1880) | 1:134:A:TRP:HA | 1:142:A:ILE:HG22 | 5 | 0.13 |
| (1,1880) | 1:134:A:TRP:HA | 1:142:A:ILE:HG23 | 5 | 0.13 |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB | 4 | 0.13 |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB | 4 | 0.13 |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB | 4 | 0.13 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 2 | 0.13 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 9 | 0.13 |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H | 6 | 0.13 |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H | 6 | 0.13 |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H | 6 | 0.13 |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H | 8 | 0.13 |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H | 8 | 0.13 |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H | 8 | 0.13 |
| (1,1799) | 1:128:A:TYR:HD1 | 1:128:A:TYR:H | 5 | 0.13 |
| (1,1799) | 1:128:A:TYR:HD2 | 1:128:A:TYR:H | 5 | 0.13 |
| (1,1723) | 1:116:A:GLU:HG2 | 1:116:A:GLU:H | 8 | 0.13 |
| (1,1723) | 1:116:A:GLU:HG3 | 1:116:A:GLU:H | 8 | 0.13 |
| (1,1702) | 1:115:A:LYS:HB2 | 1:116:A:GLU:H | 5 | 0.13 |
| (1,1690) | 1:115:A:LYS:HA | 1:115:A:LYS:HG2 | 7 | 0.13 |
| (1,1690) | 1:115:A:LYS:HA | 1:115:A:LYS:HG3 | 7 | 0.13 |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H | 10 | 0.13 |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H | 10 | 0.13 |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H | 10 | 0.13 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 3 | 0.13 |
| (1,1505) | 1:98:A:THR:HA | 1:100:A:ALA:H | 1 | 0.13 |
| (1,1474) | 1:95:A:PHE:HB2 | 1:95:A:PHE:H | 7 | 0.13 |
| (1,1474) | 1:95:A:PHE:HB3 | 1:95:A:PHE:H | 7 | 0.13 |
| (1,1446) | 1:90:A:THR:HA | 1:93:A:GLY:H | 2 | 0.13 |
| (1,1439) | 1:88:A:ASN:H | 1:134:A:TRP:HZ3 | 5 | 0.13 |
| (1,1380) | 1:87:A:THR:HA | 1:134:A:TRP:HH2 | 5 | 0.13 |
| (1,1379) | 1:87:A:THR:HA | 1:134:A:TRP:HE3 | 5 | 0.13 |
| (1,1379) | 1:87:A:THR:HA | 1:134:A:TRP:HE3 | 8 | 0.13 |
| (1,1371) | 1:86:A:GLU:H | 1:134:A:TRP:HE1 | 3 | 0.13 |
| (1,1371) | 1:86:A:GLU:H | 1:134:A:TRP:HE1 | 4 | 0.13 |
| (1,1371) | 1:86:A:GLU:H | 1:134:A:TRP:HE1 | 10 | 0.13 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG21 | 1 | 0.13 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG22 | 1 | 0.13 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG23 | 1 | 0.13 |
| (1,1363) | 1:86:A:GLU:HG3 | 1:86:A:GLU:H | 3 | 0.13 |
| (1,1363) | 1:86:A:GLU:HG3 | 1:86:A:GLU:H | 6 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 3 | 0.13 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 3 | 0.13 |
| (1,1333) | 1:85:A:TYR:HA | 1:86:A:GLU:H | 4 | 0.13 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 4 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 2 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 2 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 2 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 2 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 2 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 2 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 4 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 4 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 4 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 4 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 4 | 0.13 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 4 | 0.13 |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H | 8 | 0.13 |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H | 8 | 0.13 |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H | 8 | 0.13 |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H | 10 | 0.13 |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H | 10 | 0.13 |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H | 10 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 5 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 5 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 5 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 5 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 5 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 5 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 5 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 5 | 0.13 |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 5 | 0.13 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 4 | 0.13 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 5 | 0.13 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 6 | 0.13 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 8 | 0.13 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 10 | 0.13 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 8 | 0.13 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 8 | 0.13 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 8 | 0.13 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 8 | 0.13 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 8 | 0.13 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 8 | 0.13 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 8 | 0.13 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 8 | 0.13 |
| (1,1127) | 1:78:A:GLN:H | 1:104:A:LEU:H | 2 | 0.13 |
| (1,1127) | 1:78:A:GLN:H | 1:104:A:LEU:H | 4 | 0.13 |
| (1,1127) | 1:78:A:GLN:H | 1:104:A:LEU:H | 10 | 0.13 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 2 | 0.13 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 2 | 0.13 |
| (1,922) | 1:70:A:LEU:HD11 | 1:70:A:LEU:H | 2 | 0.13 |
| (1,922) | 1:70:A:LEU:HD12 | 1:70:A:LEU:H | 2 | 0.13 |
| (1,922) | 1:70:A:LEU:HD13 | 1:70:A:LEU:H | 2 | 0.13 |
| (1,894) | 1:68:A:GLU:H | 1:69:A:GLN:H | 1 | 0.13 |
| (1,857) | 1:66:A:ASN:HD22 | 1:174:A:ILE:H | 5 | 0.13 |
| (1,857) | 1:66:A:ASN:HD22 | 1:174:A:ILE:H | 6 | 0.13 |
| (1,834) | 1:66:A:ASN:HB3 | 1:66:A:ASN:H | 3 | 0.13 |
| (1,834) | 1:66:A:ASN:HB3 | 1:66:A:ASN:H | 4 | 0.13 |
| (1,834) | 1:66:A:ASN:HB3 | 1:66:A:ASN:H | 10 | 0.13 |
| (1,831) | 1:66:A:ASN:HA | 1:174:A:ILE:HB | 4 | 0.13 |
| (1,831) | 1:66:A:ASN:HA | 1:174:A:ILE:HB | 5 | 0.13 |
| (1,795) | 1:64:A:LEU:HG | 1:67:A:ALA:HA | 10 | 0.13 |
| (1,761) | 1:63:A:THR:H | 1:175:A:PHE:HA | 1 | 0.13 |
| (1,643) | 1:57:A:ASP:HB2 | 1:115:A:LYS:H | 9 | 0.13 |
| (1,623) | 1:55:A:VAL:H | 1:115:A:LYS:HA | 1 | 0.13 |
| (1,554) | 1:50:A:TRP:HD1 | 1:50:A:TRP:H | 1 | 0.13 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 4 | 0.13 |
| (1,553) | 1:50:A:TRP:HB2 | 1:52:A:LYS:H | 6 | 0.13 |
| (1,548) | 1:50:A:TRP:HB3 | 1:50:A:TRP:H | 4 | 0.13 |
| (1,548) | 1:50:A:TRP:HB3 | 1:50:A:TRP:H | 7 | 0.13 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 5 | 0.13 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 5 | 0.13 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 5 | 0.13 |
| (1,503) | 1:48:A:ILE:HG21 | 1:143:A:ILE:HG21 | 10 | 0.13 |
| (1,503) | 1:48:A:ILE:HG21 | 1:143:A:ILE:HG22 | 10 | 0.13 |
| (1,503) | 1:48:A:ILE:HG21 | 1:143:A:ILE:HG23 | 10 | 0.13 |
| (1,503) | 1:48:A:ILE:HG22 | 1:143:A:ILE:HG21 | 10 | 0.13 |
| (1,503) | 1:48:A:ILE:HG22 | 1:143:A:ILE:HG22 | 10 | 0.13 |
| (1,503) | 1:48:A:ILE:HG22 | 1:143:A:ILE:HG23 | 10 | 0.13 |
| (1,503) | 1:48:A:ILE:HG23 | 1:143:A:ILE:HG21 | 10 | 0.13 |
| (1,503) | 1:48:A:ILE:HG23 | 1:143:A:ILE:HG22 | 10 | 0.13 |
| (1,503) | 1:48:A:ILE:HG23 | 1:143:A:ILE:HG23 | 10 | 0.13 |
| (1,480) | 1:48:A:ILE:HB | 1:50:A:TRP:HE1 | 5 | 0.13 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG21 | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG22 | 2 | 0.13 |
| (1,436) | 1:46:A:TYR:HB2 | 1:153:A:ILE:HG23 | 2 | 0.13 |
| (1,432) | 1:46:A:TYR:HB3 | 1:154:A:LEU:H | 1 | 0.13 |
| (1,426) | 1:46:A:TYR:HA | 1:156:A:PHE:HA | 6 | 0.13 |
| (1,426) | 1:46:A:TYR:HA | 1:156:A:PHE:HA | 7 | 0.13 |
| (1,424) | 1:46:A:TYR:HA | 1:155:A:ASN:HB2 | 3 | 0.13 |
| (1,259) | 1:33:A:THR:HB | 1:35:A:ALA:H | 5 | 0.13 |
| (1,259) | 1:33:A:THR:HB | 1:35:A:ALA:H | 6 | 0.13 |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE1 | 5 | 0.13 |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE2 | 5 | 0.13 |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE1 | 5 | 0.13 |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE2 | 5 | 0.13 |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE1 | 5 | 0.13 |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE2 | 5 | 0.13 |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H | 2 | 0.13 |
| (1,235) | 1:32:A:ILE:HG22 | 1:33:A:THR:H | 2 | 0.13 |
| (1,235) | 1:32:A:ILE:HG23 | 1:33:A:THR:H | 2 | 0.13 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 2 | 0.13 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 3 | 0.13 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 7 | 0.13 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 10 | 0.13 |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H | 2 | 0.13 |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H | 5 | 0.13 |
| (1,220) | 1:32:A:ILE:HD11 | 1:158:A:ALA:HB1 | 9 | 0.13 |
| (1,220) | 1:32:A:ILE:HD11 | 1:158:A:ALA:HB2 | 9 | 0.13 |
| (1,220) | 1:32:A:ILE:HD11 | 1:158:A:ALA:HB3 | 9 | 0.13 |
| (1,220) | 1:32:A:ILE:HD12 | 1:158:A:ALA:HB1 | 9 | 0.13 |
| (1,220) | 1:32:A:ILE:HD12 | 1:158:A:ALA:HB2 | 9 | 0.13 |
| (1,220) | 1:32:A:ILE:HD12 | 1:158:A:ALA:HB3 | 9 | 0.13 |
| (1,220) | 1:32:A:ILE:HD13 | 1:158:A:ALA:HB1 | 9 | 0.13 |
| (1,220) | 1:32:A:ILE:HD13 | 1:158:A:ALA:HB2 | 9 | 0.13 |
| (1,220) | 1:32:A:ILE:HD13 | 1:158:A:ALA:HB3 | 9 | 0.13 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 7 | 0.13 |
| (1,32) | 1:23:A:ILE:HG12 | 1:23:A:ILE:H | 10 | 0.13 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG21 | 4 | 0.13 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG22 | 4 | 0.13 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG23 | 4 | 0.13 |
| (1,12) | 1:21:A:GLU:HA | 1:21:A:GLU:HG2 | 6 | 0.13 |
| (1,12) | 1:21:A:GLU:HA | 1:21:A:GLU:HG3 | 6 | 0.13 |
| (1,12) | 1:21:A:GLU:HA | 1:21:A:GLU:HG2 | 9 | 0.13 |
| (1,12) | 1:21:A:GLU:HA | 1:21:A:GLU:HG3 | 9 | 0.13 |
| (4,21) | 1:59:A:LYS:O | 1:180:A:LEU:H | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,2) | 1:33:A:THR:HA | 1:34:A:PRO:HD3 | 8 | 0.12 |
| (2,761) | 1:168:A:PHE:H | 1:169:A:ASP:H | 5 | 0.12 |
| (2,761) | 1:168:A:PHE:H | 1:169:A:ASP:H | 8 | 0.12 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE1 | 8 | 0.12 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE2 | 8 | 0.12 |
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE1 | 10 | 0.12 |
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE2 | 10 | 0.12 |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE1 | 10 | 0.12 |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE2 | 10 | 0.12 |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE1 | 10 | 0.12 |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE2 | 10 | 0.12 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 5 | 0.12 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 5 | 0.12 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2 | 8 | 0.12 |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3 | 8 | 0.12 |
| (2,443) | 1:76:A:TYR:HE1 | 1:78:A:GLN:HE22 | 4 | 0.12 |
| (2,443) | 1:76:A:TYR:HE2 | 1:78:A:GLN:HE22 | 4 | 0.12 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE1 | 3 | 0.12 |
| (2,425) | 1:74:A:PHE:HZ | 1:160:A:TYR:HE2 | 3 | 0.12 |
| (2,178) | 1:36:A:ALA:H | 1:37:A:GLY:H | 1 | 0.12 |
| (2,94) | 1:23:A:ILE:HD11 | 1:53:A:ASP:H | 1 | 0.12 |
| (2,94) | 1:23:A:ILE:HD12 | 1:53:A:ASP:H | 1 | 0.12 |
| (2,94) | 1:23:A:ILE:HD13 | 1:53:A:ASP:H | 1 | 0.12 |
| (2,27) | 1:19:A:VAL:H | 1:20:A:SER:H | 4 | 0.12 |
| (2,26) | 1:19:A:VAL:H | 1:20:A:SER:HB2 | 5 | 0.12 |
| (2,26) | 1:19:A:VAL:H | 1:20:A:SER:HB3 | 5 | 0.12 |
| (2,26) | 1:19:A:VAL:H | 1:20:A:SER:HB2 | 7 | 0.12 |
| (2,26) | 1:19:A:VAL:H | 1:20:A:SER:HB3 | 7 | 0.12 |
| (1,2270) | 1:166:A:MET:HA | 1:167:A:LEU:H | 10 | 0.12 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 6 | 0.12 |
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 4 | 0.12 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 9 | 0.12 |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 9 | 0.12 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 9 | 0.12 |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 9 | 0.12 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 9 | 0.12 |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 9 | 0.12 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 7 | 0.12 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 7 | 0.12 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 7 | 0.12 |
| (1,2054) | 1:145:A:TYR:HD1 | 1:146:A:ASN:H | 10 | 0.12 |
| (1,2054) | 1:145:A:TYR:HD2 | 1:146:A:ASN:H | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2 | 4 | 0.12 |
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2 | 5 | 0.12 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 10 | 0.12 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 3 | 0.12 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 5 | 0.12 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 6 | 0.12 |
| (1,1817) | 1:131:A:THR:HB | 1:132:A:SER:H | 3 | 0.12 |
| (1,1817) | 1:131:A:THR:HB | 1:132:A:SER:H | 10 | 0.12 |
| (1,1794) | 1:128:A:TYR:HA | 1:128:A:TYR:HB2 | 3 | 0.12 |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H | 2 | 0.12 |
| (1,1778) | 1:121:A:LEU:HG | 1:121:A:LEU:H | 4 | 0.12 |
| (1,1778) | 1:121:A:LEU:HG | 1:121:A:LEU:H | 6 | 0.12 |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H | 7 | 0.12 |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H | 7 | 0.12 |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H | 7 | 0.12 |
| (1,1723) | 1:116:A:GLU:HG2 | 1:116:A:GLU:H | 4 | 0.12 |
| (1,1723) | 1:116:A:GLU:HG3 | 1:116:A:GLU:H | 4 | 0.12 |
| (1,1723) | 1:116:A:GLU:HG2 | 1:116:A:GLU:H | 9 | 0.12 |
| (1,1723) | 1:116:A:GLU:HG3 | 1:116:A:GLU:H | 9 | 0.12 |
| (1,1681) | 1:114:A:ASP:HB2 | 1:116:A:GLU:H | 6 | 0.12 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 4 | 0.12 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD21 | 5 | 0.12 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD22 | 5 | 0.12 |
| (1,1653) | 1:113:A:LEU:HA | 1:113:A:LEU:HD23 | 5 | 0.12 |
| (1,1629) | 1:110:A:VAL:HG11 | 1:111:A:ILE:H | 1 | 0.12 |
| (1,1629) | 1:110:A:VAL:HG12 | 1:111:A:ILE:H | 1 | 0.12 |
| (1,1629) | 1:110:A:VAL:HG13 | 1:111:A:ILE:H | 1 | 0.12 |
| (1,1574) | 1:104:A:LEU:HG | 1:104:A:LEU:H | 7 | 0.12 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 8 | 0.12 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 10 | 0.12 |
| (1,1505) | 1:98:A:THR:HA | 1:100:A:ALA:H | 10 | 0.12 |
| (1,1432) | 1:88:A:ASN:H | 1:89:A:SER:H | 9 | 0.12 |
| (1,1422) | 1:88:A:ASN:HB2 | 1:88:A:ASN:HD21 | 6 | 0.12 |
| (1,1422) | 1:88:A:ASN:HB2 | 1:88:A:ASN:HD21 | 10 | 0.12 |
| (1,1379) | 1:87:A:THR:HA | 1:134:A:TRP:HE3 | 9 | 0.12 |
| (1,1371) | 1:86:A:GLU:H | 1:134:A:TRP:HE1 | 8 | 0.12 |
| (1,1333) | 1:85:A:TYR:HA | 1:86:A:GLU:H | 8 | 0.12 |
| (1,1317) | 1:83:A:SER:H | 1:99:A:LYS:H | 2 | 0.12 |
| (1,1282) | 1:82:A:THR:H | 1:155:A:ASN:HB3 | 8 | 0.12 |
| (1,1282) | 1:82:A:THR:H | 1:155:A:ASN:HB3 | 10 | 0.12 |
| (1,1271) | 1:82:A:THR:HG21 | 1:83:A:SER:H | 9 | 0.12 |
| (1,1271) | 1:82:A:THR:HG22 | 1:83:A:SER:H | 9 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1271) | 1:82:A:THR:HG23 | 1:83:A:SER:H | 9 | 0.12 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 8 | 0.12 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 10 | 0.12 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 8 | 0.12 |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 8 | 0.12 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 8 | 0.12 |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 8 | 0.12 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 8 | 0.12 |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 8 | 0.12 |
| (1,1207) | 1:81:A:ILE:HA | 1:82:A:THR:H | 1 | 0.12 |
| (1,1086) | 1:77:A:LEU:HB2 | 1:78:A:GLN:H | 5 | 0.12 |
| (1,1086) | 1:77:A:LEU:HB2 | 1:78:A:GLN:H | 6 | 0.12 |
| (1,1055) | 1:76:A:TYR:HB3 | 1:77:A:LEU:H | 10 | 0.12 |
| (1,1004) | 1:74:A:PHE:HA | 1:162:A:ALA:HA | 4 | 0.12 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 3 | 0.12 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 4 | 0.12 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 5 | 0.12 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 9 | 0.12 |
| (1,914) | 1:69:A:GLN:HG3 | 1:69:A:GLN:H | 10 | 0.12 |
| (1,881) | 1:68:A:GLU:HA | 1:68:A:GLU:HG2 | 1 | 0.12 |
| (1,863) | 1:66:A:ASN:H | 1:175:A:PHE:HA | 9 | 0.12 |
| (1,795) | 1:64:A:LEU:HG | 1:67:A:ALA:HA | 2 | 0.12 |
| (1,795) | 1:64:A:LEU:HG | 1:67:A:ALA:HA | 6 | 0.12 |
| (1,761) | 1:63:A:THR:H | 1:175:A:PHE:HA | 2 | 0.12 |
| (1,735) | 1:62:A:VAL:H | 1:108:A:SER:HA | 4 | 0.12 |
| (1,683) | 1:60:A:LEU:HG | 1:60:A:LEU:H | 2 | 0.12 |
| (1,683) | 1:60:A:LEU:HG | 1:60:A:LEU:H | 7 | 0.12 |
| (1,643) | 1:57:A:ASP:HB2 | 1:115:A:LYS:H | 3 | 0.12 |
| (1,643) | 1:57:A:ASP:HB2 | 1:115:A:LYS:H | 7 | 0.12 |
| (1,643) | 1:57:A:ASP:HB2 | 1:115:A:LYS:H | 10 | 0.12 |
| (1,640) | 1:57:A:ASP:HB3 | 1:115:A:LYS:H | 6 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 4 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 4 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 4 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 6 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 6 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 6 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG21 | 7 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG22 | 7 | 0.12 |
| (1,568) | 1:51:A:ILE:HA | 1:51:A:ILE:HG23 | 7 | 0.12 |
| (1,567) | 1:50:A:TRP:HZ3 | 1:151:A:VAL:HG21 | 10 | 0.12 |
| (1,567) | 1:50:A:TRP:HZ3 | 1:151:A:VAL:HG22 | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,567) | 1:50:A:TRP:HZ3 | 1:151:A:VAL:HG23 | 10 | 0.12 |
| (1,548) | 1:50:A:TRP:HB3 | 1:50:A:TRP:H | 1 | 0.12 |
| (1,548) | 1:50:A:TRP:HB3 | 1:50:A:TRP:H | 2 | 0.12 |
| (1,548) | 1:50:A:TRP:HB3 | 1:50:A:TRP:H | 3 | 0.12 |
| (1,548) | 1:50:A:TRP:HB3 | 1:50:A:TRP:H | 8 | 0.12 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 2 | 0.12 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 2 | 0.12 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 2 | 0.12 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 9 | 0.12 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 9 | 0.12 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 9 | 0.12 |
| (1,426) | 1:46:A:TYR:HA | 1:156:A:PHE:HA | 3 | 0.12 |
| (1,424) | 1:46:A:TYR:HA | 1:155:A:ASN:HB2 | 6 | 0.12 |
| (1,292) | 1:37:A:GLY:HA2 | 1:37:A:GLY:H | 5 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 1 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 2 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 3 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 4 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 5 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 6 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 7 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 8 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 9 | 0.12 |
| (1,291) | 1:37:A:GLY:HA2 | 1:37:A:GLY:HA3 | 10 | 0.12 |
| (1,272) | 1:34:A:PRO:HD2 | 1:35:A:ALA:H | 1 | 0.12 |
| (1,272) | 1:34:A:PRO:HD2 | 1:35:A:ALA:H | 9 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 2 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 2 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 2 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 4 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 4 | 0.12 |
| (1,254) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 4 | 0.12 |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H | 6 | 0.12 |
| (1,202) | 1:31:A:SER:HB2 | 1:173:A:VAL:H | 1 | 0.12 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 7 | 0.12 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 7 | 0.12 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 7 | 0.12 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 7 | 0.12 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 7 | 0.12 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 7 | 0.12 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 7 | 0.12 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 7 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 7 | 0.12 |
| (1,77) | 1:25:A:VAL:HG11 | 1:25:A:VAL:H | 2 | 0.12 |
| (1,77) | 1:25:A:VAL:HG12 | 1:25:A:VAL:H | 2 | 0.12 |
| (1,77) | 1:25:A:VAL:HG13 | 1:25:A:VAL:H | 2 | 0.12 |
| (1,77) | 1:25:A:VAL:HG11 | 1:25:A:VAL:H | 8 | 0.12 |
| (1,77) | 1:25:A:VAL:HG12 | 1:25:A:VAL:H | 8 | 0.12 |
| (1,77) | 1:25:A:VAL:HG13 | 1:25:A:VAL:H | 8 | 0.12 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 5 | 0.12 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 9 | 0.12 |
| (1,48) | 1:24:A:ASP:HB3 | 1:50:A:TRP:HD1 | 5 | 0.12 |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H | 3 | 0.11 |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H | 3 | 0.11 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE1 | 5 | 0.11 |
| (2,518) | 1:84:A:GLY:HA2 | 1:95:A:PHE:HE2 | 5 | 0.11 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE1 | 5 | 0.11 |
| (2,518) | 1:84:A:GLY:HA3 | 1:95:A:PHE:HE2 | 5 | 0.11 |
| (2,397) | 1:73:A:TYR:HD1 | 1:74:A:PHE:HA | 4 | 0.11 |
| (2,397) | 1:73:A:TYR:HD2 | 1:74:A:PHE:HA | 4 | 0.11 |
| (2,389) | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 1 | 0.11 |
| (2,389) | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 1 | 0.11 |
| (2,389) | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 1 | 0.11 |
| (2,178) | 1:36:A:ALA:H | 1:37:A:GLY:H | 3 | 0.11 |
| (2,123) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 1 | 0.11 |
| (2,123) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 1 | 0.11 |
| (2,123) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE1 | 7 | 0.11 |
| (2,123) | 1:28:A:HIS:HD2 | 1:46:A:TYR:HE2 | 7 | 0.11 |
| (1,2459) | 1:182:A:VAL:HB | 1:183:A:GLY:H | 3 | 0.11 |
| (1,2459) | 1:182:A:VAL:HB | 1:183:A:GLY:H | 4 | 0.11 |
| (1,2459) | 1:182:A:VAL:HB | 1:183:A:GLY:H | 5 | 0.11 |
| (1,2425) | 1:177:A:PHE:HD1 | 1:177:A:PHE:H | 8 | 0.11 |
| (1,2425) | 1:177:A:PHE:HD2 | 1:177:A:PHE:H | 8 | 0.11 |
| (1,2316) | 1:171:A:LEU:HA | 1:172:A:PRO:HD3 | 9 | 0.11 |
| (1,2295) | 1:169:A:ASP:HB3 | 1:170:A:SER:H | 1 | 0.11 |
| (1,2276) | 1:167:A:LEU:H | 1:168:A:PHE:H | 10 | 0.11 |
| (1,2275) | 1:167:A:LEU:HA | 1:168:A:PHE:H | 3 | 0.11 |
| (1,2275) | 1:167:A:LEU:HA | 1:168:A:PHE:H | 5 | 0.11 |
| (1,2271) | 1:166:A:MET:HB3 | 1:167:A:LEU:H | 8 | 0.11 |
| (1,2260) | 1:163:A:LYS:H | 1:168:A:PHE:HZ | 10 | 0.11 |
| (1,2258) | 1:163:A:LYS:HG2 | 1:163:A:LYS:H | 7 | 0.11 |
| (1,2257) | 1:163:A:LYS:HG3 | 1:163:A:LYS:H | 9 | 0.11 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 1 | 0.11 |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 2 | 0.11 |
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 3 | 0.11 |
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 7 | 0.11 |
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 8 | 0.11 |
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 10 | 0.11 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 8 | 0.11 |
| (1,2139) | 1:155:A:ASN:H | 1:156:A:PHE:HZ | 10 | 0.11 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 4 | 0.11 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 4 | 0.11 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 4 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB1 | 6 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB2 | 6 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB3 | 6 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB1 | 7 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB2 | 7 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB3 | 7 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB1 | 10 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB2 | 10 | 0.11 |
| (1,2086) | 1:152:A:ALA:HA | 1:152:A:ALA:HB3 | 10 | 0.11 |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H | 8 | 0.11 |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H | 8 | 0.11 |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H | 8 | 0.11 |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H | 3 | 0.11 |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H | 3 | 0.11 |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H | 3 | 0.11 |
| (1,1974) | 1:138:A:GLU:H | 1:139:A:PRO:HD2 | 1 | 0.11 |
| (1,1974) | 1:138:A:GLU:H | 1:139:A:PRO:HD2 | 5 | 0.11 |
| (1,1974) | 1:138:A:GLU:H | 1:139:A:PRO:HD2 | 7 | 0.11 |
| (1,1974) | 1:138:A:GLU:H | 1:139:A:PRO:HD2 | 9 | 0.11 |
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2 | 2 | 0.11 |
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2 | 3 | 0.11 |
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2 | 10 | 0.11 |
| (1,1917) | 1:134:A:TRP:HE1 | 1:136:A:PRO:HA | 1 | 0.11 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 3 | 0.11 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 6 | 0.11 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 1 | 0.11 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 7 | 0.11 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 8 | 0.11 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 10 | 0.11 |
| (1,1778) | 1:121:A:LEU:HG | 1:121:A:LEU:H | 3 | 0.11 |
| (1,1778) | 1:121:A:LEU:HG | 1:121:A:LEU:H | 10 | 0.11 |
| (1,1761) | 1:119:A:ALA:H | 1:151:A:VAL:H | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1734) | 1:117:A:ASP:H | 1:118:A:ILE:HB | 10 | 0.11 |
| (1,1723) | 1:116:A:GLU:HG2 | 1:116:A:GLU:H | 1 | 0.11 |
| (1,1723) | 1:116:A:GLU:HG3 | 1:116:A:GLU:H | 1 | 0.11 |
| (1,1699) | 1:115:A:LYS:HB3 | 1:115:A:LYS:H | 4 | 0.11 |
| (1,1690) | 1:115:A:LYS:HA | 1:115:A:LYS:HG2 | 9 | 0.11 |
| (1,1690) | 1:115:A:LYS:HA | 1:115:A:LYS:HG3 | 9 | 0.11 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 1 | 0.11 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 5 | 0.11 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 8 | 0.11 |
| (1,1629) | 1:110:A:VAL:HG11 | 1:111:A:ILE:H | 9 | 0.11 |
| (1,1629) | 1:110:A:VAL:HG12 | 1:111:A:ILE:H | 9 | 0.11 |
| (1,1629) | 1:110:A:VAL:HG13 | 1:111:A:ILE:H | 9 | 0.11 |
| (1,1629) | 1:110:A:VAL:HG11 | 1:111:A:ILE:H | 10 | 0.11 |
| (1,1629) | 1:110:A:VAL:HG12 | 1:111:A:ILE:H | 10 | 0.11 |
| (1,1629) | 1:110:A:VAL:HG13 | 1:111:A:ILE:H | 10 | 0.11 |
| (1,1618) | 1:108:A:SER:H | 1:109:A:ALA:H | 1 | 0.11 |
| (1,1618) | 1:108:A:SER:H | 1:109:A:ALA:H | 7 | 0.11 |
| (1,1618) | 1:108:A:SER:H | 1:109:A:ALA:H | 8 | 0.11 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 2 | 0.11 |
| (1,1531) | 1:102:A:ILE:HB | 1:102:A:ILE:HG21 | 4 | 0.11 |
| (1,1531) | 1:102:A:ILE:HB | 1:102:A:ILE:HG22 | 4 | 0.11 |
| (1,1531) | 1:102:A:ILE:HB | 1:102:A:ILE:HG23 | 4 | 0.11 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 2 | 0.11 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 2 | 0.11 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 2 | 0.11 |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H | 7 | 0.11 |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H | 7 | 0.11 |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H | 7 | 0.11 |
| (1,1380) | 1:87:A:THR:HA | 1:134:A:TRP:HH2 | 8 | 0.11 |
| (1,1379) | 1:87:A:THR:HA | 1:134:A:TRP:HE3 | 1 | 0.11 |
| (1,1379) | 1:87:A:THR:HA | 1:134:A:TRP:HE3 | 4 | 0.11 |
| (1,1371) | 1:86:A:GLU:H | 1:134:A:TRP:HE1 | 1 | 0.11 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG21 | 3 | 0.11 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG22 | 3 | 0.11 |
| (1,1369) | 1:86:A:GLU:H | 1:133:A:ILE:HG23 | 3 | 0.11 |
| (1,1363) | 1:86:A:GLU:HG3 | 1:86:A:GLU:H | 4 | 0.11 |
| (1,1343) | 1:85:A:TYR:HE1 | 1:152:A:ALA:HA | 9 | 0.11 |
| (1,1343) | 1:85:A:TYR:HE2 | 1:152:A:ALA:HA | 9 | 0.11 |
| (1,1315) | 1:83:A:SER:H | 1:99:A:LYS:HG3 | 9 | 0.11 |
| (1,1271) | 1:82:A:THR:HG21 | 1:83:A:SER:H | 2 | 0.11 |
| (1,1271) | 1:82:A:THR:HG22 | 1:83:A:SER:H | 2 | 0.11 |
| (1,1271) | 1:82:A:THR:HG23 | 1:83:A:SER:H | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 1 | 0.11 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 7 | 0.11 |
| (1,1232) | 1:81:A:ILE:HG21 | 1:99:A:LYS:H | 7 | 0.11 |
| (1,1232) | 1:81:A:ILE:HG22 | 1:99:A:LYS:H | 7 | 0.11 |
| (1,1232) | 1:81:A:ILE:HG23 | 1:99:A:LYS:H | 7 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 1 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 1 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 1 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 1 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 1 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 1 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 1 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 1 | 0.11 |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 1 | 0.11 |
| (1,1128) | 1:78:A:GLN:H | 1:158:A:ALA:HA | 6 | 0.11 |
| (1,1127) | 1:78:A:GLN:H | 1:104:A:LEU:H | 1 | 0.11 |
| (1,1100) | 1:77:A:LEU:HG | 1:78:A:GLN:H | 8 | 0.11 |
| (1,1078) | 1:77:A:LEU:HA | 1:77:A:LEU:HB2 | 4 | 0.11 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 2 | 0.11 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 4 | 0.11 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 6 | 0.11 |
| (1,1075) | 1:76:A:TYR:H | 1:162:A:ALA:HA | 7 | 0.11 |
| (1,1037) | 1:74:A:PHE:HZ | 1:162:A:ALA:HA | 5 | 0.11 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 9 | 0.11 |
| (1,975) | 1:73:A:TYR:HA | 1:73:A:TYR:HB3 | 6 | 0.11 |
| (1,921) | 1:70:A:LEU:HA | 1:73:A:TYR:HD1 | 8 | 0.11 |
| (1,921) | 1:70:A:LEU:HA | 1:73:A:TYR:HD2 | 8 | 0.11 |
| (1,894) | 1:68:A:GLU:H | 1:69:A:GLN:H | 7 | 0.11 |
| (1,886) | 1:68:A:GLU:HA | 1:71:A:LYS:HD2 | 7 | 0.11 |
| (1,886) | 1:68:A:GLU:HA | 1:71:A:LYS:HD3 | 7 | 0.11 |
| (1,857) | 1:66:A:ASN:HD22 | 1:174:A:ILE:H | 4 | 0.11 |
| (1,854) | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3 | 4 | 0.11 |
| (1,854) | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3 | 8 | 0.11 |
| (1,845) | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA | 7 | 0.11 |
| (1,834) | 1:66:A:ASN:HB3 | 1:66:A:ASN:H | 5 | 0.11 |
| (1,830) | 1:66:A:ASN:HA | 1:69:A:GLN:H | 10 | 0.11 |
| (1,828) | 1:66:A:ASN:HA | 1:69:A:GLN:HG3 | 9 | 0.11 |
| (1,795) | 1:64:A:LEU:HG | 1:67:A:ALA:HA | 7 | 0.11 |
| (1,761) | 1:63:A:THR:H | 1:175:A:PHE:HA | 7 | 0.11 |
| (1,761) | 1:63:A:THR:H | 1:175:A:PHE:HA | 8 | 0.11 |
| (1,761) | 1:63:A:THR:H | 1:175:A:PHE:HA | 10 | 0.11 |
| (1,755) | 1:63:A:THR:HG21 | 1:108:A:SER:HA | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,755) | 1:63:A:THR:HG22 | 1:108:A:SER:HA | 7 | 0.11 |
| (1,755) | 1:63:A:THR:HG23 | 1:108:A:SER:HA | 7 | 0.11 |
| (1,755) | 1:63:A:THR:HG21 | 1:108:A:SER:HA | 8 | 0.11 |
| (1,755) | 1:63:A:THR:HG22 | 1:108:A:SER:HA | 8 | 0.11 |
| (1,755) | 1:63:A:THR:HG23 | 1:108:A:SER:HA | 8 | 0.11 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 3 | 0.11 |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 3 | 0.11 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 3 | 0.11 |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 3 | 0.11 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 3 | 0.11 |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 3 | 0.11 |
| (1,683) | 1:60:A:LEU:HG | 1:60:A:LEU:H | 10 | 0.11 |
| (1,639) | 1:57:A:ASP:HB3 | 1:58:A:VAL:H | 7 | 0.11 |
| (1,597) | 1:53:A:ASP:HB2 | 1:54:A:GLN:H | 7 | 0.11 |
| (1,597) | 1:53:A:ASP:HB3 | 1:54:A:GLN:H | 7 | 0.11 |
| (1,554) | 1:50:A:TRP:HD1 | 1:50:A:TRP:H | 3 | 0.11 |
| (1,548) | 1:50:A:TRP:HB3 | 1:50:A:TRP:H | 9 | 0.11 |
| (1,541) | 1:50:A:TRP:HA | 1:51:A:ILE:HB | 3 | 0.11 |
| (1,529) | 1:49:A:VAL:H | 1:151:A:VAL:HA | 7 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 3 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 3 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 3 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 4 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 4 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 4 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 8 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 8 | 0.11 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 8 | 0.11 |
| (1,493) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HA | 6 | 0.11 |
| (1,493) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HA | 6 | 0.11 |
| (1,493) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HA | 6 | 0.11 |
| (1,447) | 1:46:A:TYR:HE1 | 1:141:A:LYS:HG3 | 9 | 0.11 |
| (1,447) | 1:46:A:TYR:HE2 | 1:141:A:LYS:HG3 | 9 | 0.11 |
| (1,432) | 1:46:A:TYR:HB3 | 1:154:A:LEU:H | 2 | 0.11 |
| (1,424) | 1:46:A:TYR:HA | 1:155:A:ASN:HB2 | 5 | 0.11 |
| (1,356) | 1:42:A:ASP:HB2 | 1:160:A:TYR:HE1 | 8 | 0.11 |
| (1,356) | 1:42:A:ASP:HB2 | 1:160:A:TYR:HE2 | 8 | 0.11 |
| (1,356) | 1:42:A:ASP:HB3 | 1:160:A:TYR:HE1 | 8 | 0.11 |
| (1,356) | 1:42:A:ASP:HB3 | 1:160:A:TYR:HE2 | 8 | 0.11 |
| (1,292) | 1:37:A:GLY:HA2 | 1:37:A:GLY:H | 6 | 0.11 |
| (1,290) | 1:37:A:GLY:HA3 | 1:38:A:ALA:H | 7 | 0.11 |
| (1,268) | 1:34:A:PRO:HD3 | 1:35:A:ALA:H | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE1 | 3 | 0.11 |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE2 | 3 | 0.11 |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE1 | 3 | 0.11 |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE2 | 3 | 0.11 |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE1 | 3 | 0.11 |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE2 | 3 | 0.11 |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H | 6 | 0.11 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD11 | 6 | 0.11 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD12 | 6 | 0.11 |
| (1,190) | 1:31:A:SER:HA | 1:32:A:ILE:HD13 | 6 | 0.11 |
| (1,188) | 1:30:A:GLY:H | 1:46:A:TYR:H | 2 | 0.11 |
| (1,188) | 1:30:A:GLY:H | 1:46:A:TYR:H | 5 | 0.11 |
| (1,166) | 1:29:A:LEU:HD11 | 1:175:A:PHE:H | 5 | 0.11 |
| (1,166) | 1:29:A:LEU:HD12 | 1:175:A:PHE:H | 5 | 0.11 |
| (1,166) | 1:29:A:LEU:HD13 | 1:175:A:PHE:H | 5 | 0.11 |
| (1,141) | 1:28:A:HIS:HD2 | 1:48:A:ILE:HA | 7 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 3 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 5 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 6 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 6 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 6 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 6 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 6 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 6 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 6 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 6 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 8 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 9 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 10 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 10 | 0.11 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 10 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 10 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 10 | 0.11 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 10 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 10 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 10 | 0.11 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 10 | 0.11 |
| (1,77) | 1:25:A:VAL:HG11 | 1:25:A:VAL:H | 5 | 0.11 |
| (1,77) | 1:25:A:VAL:HG12 | 1:25:A:VAL:H | 5 | 0.11 |
| (1,77) | 1:25:A:VAL:HG13 | 1:25:A:VAL:H | 5 | 0.11 |
| (1,51) | 1:24:A:ASP:HB2 | 1:25:A:VAL:H | 8 | 0.11 |
| (1,48) | 1:24:A:ASP:HB3 | 1:50:A:TRP:HD1 | 7 | 0.11 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG21 | 7 | 0.11 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG22 | 7 | 0.11 |
| (1,25) | 1:23:A:ILE:HA | 1:23:A:ILE:HG23 | 7 | 0.11 |
| (1,9) | 1:19:A:VAL:HB | 1:19:A:VAL:H | 5 | 0.11 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE1 | 7 | 0.1 |
| (2,732) | 1:155:A:ASN:H | 1:156:A:PHE:HE2 | 7 | 0.1 |
| (2,512) | 1:83:A:SER:HB2 | 1:154:A:LEU:HA | 6 | 0.1 |
| (2,206) | 1:39:A:GLN:HB2 | 1:39:A:GLN:HE21 | 10 | 0.1 |
| (2,27) | 1:19:A:VAL:H | 1:20:A:SER:H | 5 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2459) | 1:182:A:VAL:HB | 1:183:A:GLY:H | 2 | 0.1 |
| (1,2459) | 1:182:A:VAL:HB | 1:183:A:GLY:H | 7 | 0.1 |
| (1,2459) | 1:182:A:VAL:HB | 1:183:A:GLY:H | 10 | 0.1 |
| (1,2450) | 1:180:A:LEU:H | 1:181:A:GLN:H | 5 | 0.1 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD11 | 7 | 0.1 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD12 | 7 | 0.1 |
| (1,2303) | 1:170:A:SER:HA | 1:171:A:LEU:HD13 | 7 | 0.1 |
| (1,2299) | 1:169:A:ASP:H | 1:170:A:SER:H | 3 | 0.1 |
| (1,2299) | 1:169:A:ASP:H | 1:170:A:SER:H | 5 | 0.1 |
| (1,2295) | 1:169:A:ASP:HB3 | 1:170:A:SER:H | 6 | 0.1 |
| (1,2275) | 1:167:A:LEU:HA | 1:168:A:PHE:H | 2 | 0.1 |
| (1,2275) | 1:167:A:LEU:HA | 1:168:A:PHE:H | 4 | 0.1 |
| (1,2275) | 1:167:A:LEU:HA | 1:168:A:PHE:H | 10 | 0.1 |
| (1,2260) | 1:163:A:LYS:H | 1:168:A:PHE:HZ | 5 | 0.1 |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ | 8 | 0.1 |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ | 8 | 0.1 |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ | 8 | 0.1 |
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 1 | 0.1 |
| (1,2183) | 1:158:A:ALA:HA | 1:159:A:PHE:HB3 | 5 | 0.1 |
| (1,2124) | 1:155:A:ASN:HA | 1:155:A:ASN:HD21 | 5 | 0.1 |
| (1,2124) | 1:155:A:ASN:HA | 1:155:A:ASN:HD22 | 5 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 1 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 1 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 1 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 2 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 2 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 2 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 9 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 9 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 9 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H | 10 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 10 | 0.1 |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 10 | 0.1 |
| (1,1974) | 1:138:A:GLU:H | 1:139:A:PRO:HD2 | 6 | 0.1 |
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2 | 6 | 0.1 |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA | 9 | 0.1 |
| (1,1826) | 1:132:A:SER:HA | 1:133:A:ILE:HB | 4 | 0.1 |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H | 5 | 0.1 |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H | 7 | 0.1 |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H | 9 | 0.1 |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H | 10 | 0.1 |
| (1,1761) | 1:119:A:ALA:H | 1:151:A:VAL:H | 6 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1684) | 1:114:A:ASP:H | 1:116:A:GLU:H | 5 | 0.1 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 2 | 0.1 |
| (1,1677) | 1:114:A:ASP:HA | 1:118:A:ILE:H | 3 | 0.1 |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H | 3 | 0.1 |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H | 3 | 0.1 |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H | 3 | 0.1 |
| (1,1618) | 1:108:A:SER:H | 1:109:A:ALA:H | 3 | 0.1 |
| (1,1618) | 1:108:A:SER:H | 1:109:A:ALA:H | 5 | 0.1 |
| (1,1618) | 1:108:A:SER:H | 1:109:A:ALA:H | 6 | 0.1 |
| (1,1618) | 1:108:A:SER:H | 1:109:A:ALA:H | 10 | 0.1 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 7 | 0.1 |
| (1,1532) | 1:102:A:ILE:HB | 1:102:A:ILE:H | 9 | 0.1 |
| (1,1439) | 1:88:A:ASN:H | 1:134:A:TRP:HZ3 | 7 | 0.1 |
| (1,1436) | 1:88:A:ASN:H | 1:133:A:ILE:HA | 3 | 0.1 |
| (1,1422) | 1:88:A:ASN:HB2 | 1:88:A:ASN:HD21 | 1 | 0.1 |
| (1,1408) | 1:87:A:THR:H | 1:134:A:TRP:HH2 | 7 | 0.1 |
| (1,1380) | 1:87:A:THR:HA | 1:134:A:TRP:HH2 | 7 | 0.1 |
| (1,1365) | 1:86:A:GLU:HG2 | 1:86:A:GLU:H | 4 | 0.1 |
| (1,1250) | 1:81:A:ILE:H | 1:156:A:PHE:HA | 5 | 0.1 |
| (1,1127) | 1:78:A:GLN:H | 1:104:A:LEU:H | 5 | 0.1 |
| (1,1127) | 1:78:A:GLN:H | 1:104:A:LEU:H | 8 | 0.1 |
| (1,1020) | 1:74:A:PHE:HD1 | 1:162:A:ALA:HA | 5 | 0.1 |
| (1,1020) | 1:74:A:PHE:HD2 | 1:162:A:ALA:HA | 5 | 0.1 |
| (1,1006) | 1:74:A:PHE:HA | 1:163:A:LYS:H | 6 | 0.1 |
| (1,914) | 1:69:A:GLN:HG3 | 1:69:A:GLN:H | 2 | 0.1 |
| (1,828) | 1:66:A:ASN:HA | 1:69:A:GLN:HG3 | 10 | 0.1 |
| (1,795) | 1:64:A:LEU:HG | 1:67:A:ALA:HA | 1 | 0.1 |
| (1,795) | 1:64:A:LEU:HG | 1:67:A:ALA:HA | 4 | 0.1 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG21 | 5 | 0.1 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG22 | 5 | 0.1 |
| (1,710) | 1:62:A:VAL:HA | 1:62:A:VAL:HG23 | 5 | 0.1 |
| (1,678) | 1:60:A:LEU:HA | 1:111:A:ILE:H | 6 | 0.1 |
| (1,678) | 1:60:A:LEU:HA | 1:111:A:ILE:H | 7 | 0.1 |
| (1,678) | 1:60:A:LEU:HA | 1:111:A:ILE:H | 8 | 0.1 |
| (1,643) | 1:57:A:ASP:HB2 | 1:115:A:LYS:H | 8 | 0.1 |
| (1,639) | 1:57:A:ASP:HB3 | 1:58:A:VAL:H | 5 | 0.1 |
| (1,541) | 1:50:A:TRP:HA | 1:51:A:ILE:HB | 1 | 0.1 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG11 | 1 | 0.1 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG12 | 1 | 0.1 |
| (1,513) | 1:49:A:VAL:HA | 1:49:A:VAL:HG13 | 1 | 0.1 |
| (1,455) | 1:47:A:ALA:HB1 | 1:48:A:ILE:H | 3 | 0.1 |
| (1,455) | 1:47:A:ALA:HB2 | 1:48:A:ILE:H | 3 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,455) | 1:47:A:ALA:HB3 | 1:48:A:ILE:H | 3 | 0.1 |
| (1,454) | 1:47:A:ALA:HB1 | 1:47:A:ALA:H | 7 | 0.1 |
| (1,454) | 1:47:A:ALA:HB2 | 1:47:A:ALA:H | 7 | 0.1 |
| (1,454) | 1:47:A:ALA:HB3 | 1:47:A:ALA:H | 7 | 0.1 |
| (1,432) | 1:46:A:TYR:HB3 | 1:154:A:LEU:H | 5 | 0.1 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE1 | 10 | 0.1 |
| (1,427) | 1:46:A:TYR:HA | 1:156:A:PHE:HE2 | 10 | 0.1 |
| (1,426) | 1:46:A:TYR:HA | 1:156:A:PHE:HA | 10 | 0.1 |
| (1,356) | 1:42:A:ASP:HB2 | 1:160:A:TYR:HE1 | 9 | 0.1 |
| (1,356) | 1:42:A:ASP:HB2 | 1:160:A:TYR:HE2 | 9 | 0.1 |
| (1,356) | 1:42:A:ASP:HB3 | 1:160:A:TYR:HE1 | 9 | 0.1 |
| (1,356) | 1:42:A:ASP:HB3 | 1:160:A:TYR:HE2 | 9 | 0.1 |
| (1,290) | 1:37:A:GLY:HA3 | 1:38:A:ALA:H | 4 | 0.1 |
| (1,272) | 1:34:A:PRO:HD2 | 1:35:A:ALA:H | 3 | 0.1 |
| (1,256) | 1:33:A:THR:HA | 1:168:A:PHE:HZ | 5 | 0.1 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG21 | 10 | 0.1 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG22 | 10 | 0.1 |
| (1,209) | 1:32:A:ILE:HA | 1:32:A:ILE:HG23 | 10 | 0.1 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 7 | 0.1 |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 7 | 0.1 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 7 | 0.1 |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 7 | 0.1 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 7 | 0.1 |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 7 | 0.1 |
| (1,141) | 1:28:A:HIS:HD2 | 1:48:A:ILE:HA | 2 | 0.1 |
| (1,92) | 1:25:A:VAL:H | 1:50:A:TRP:HE1 | 6 | 0.1 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 4 | 0.1 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 4 | 0.1 |
| (1,82) | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 4 | 0.1 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 4 | 0.1 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 4 | 0.1 |
| (1,82) | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 4 | 0.1 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 4 | 0.1 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 4 | 0.1 |
| (1,82) | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 4 | 0.1 |
| (1,54) | 1:24:A:ASP:HB2 | 1:50:A:TRP:HB2 | 2 | 0.1 |

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

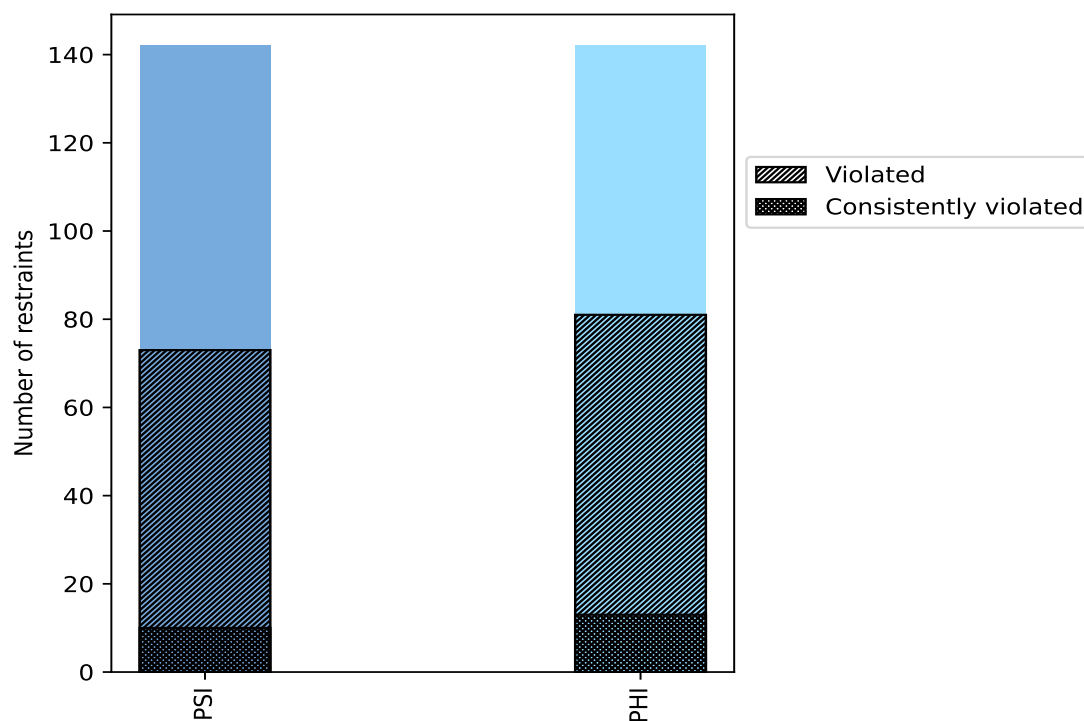
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PSI | 142 | 50.0 | 73 | 51.4 | 25.7 | 10 | 7.0 | 3.5 |
| PHI | 142 | 50.0 | 81 | 57.0 | 28.5 | 13 | 9.2 | 4.6 |
| Total | 284 | 100.0 | 154 | 54.2 | 54.2 | 23 | 8.1 | 8.1 |

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

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



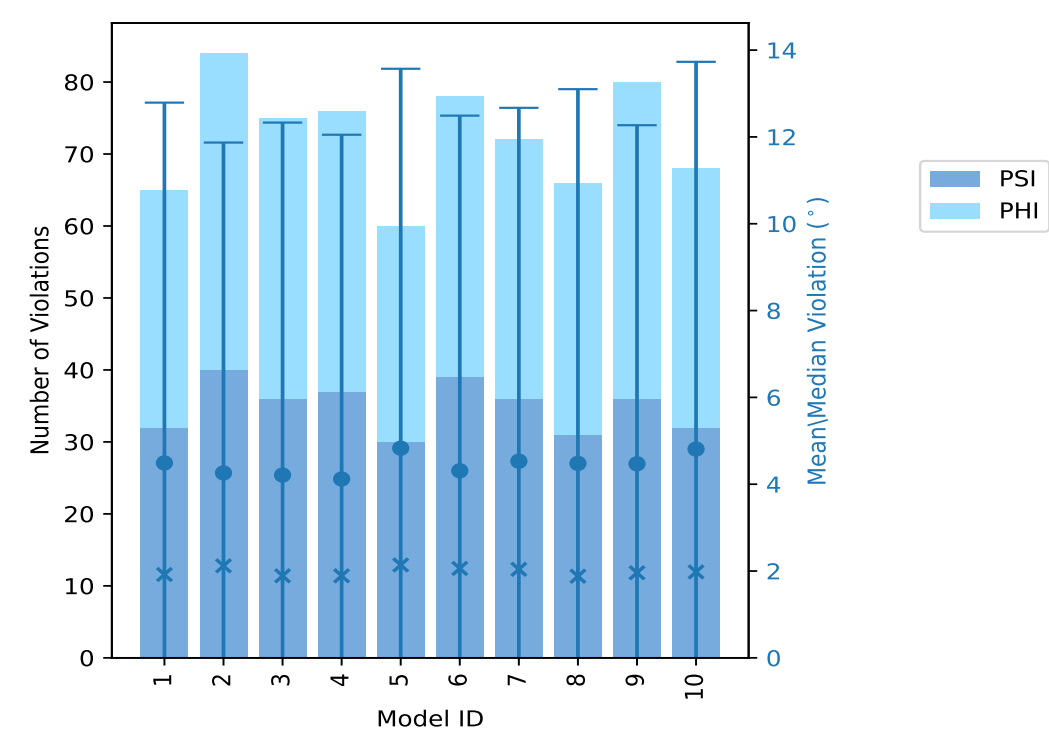
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PSI | PHI | Total | | | | |
| 1 | 32 | 33 | 65 | 4.49 | 40.03 | 8.3 | 1.92 |
| 2 | 40 | 44 | 84 | 4.26 | 39.91 | 7.61 | 2.12 |
| 3 | 36 | 39 | 75 | 4.21 | 40.34 | 8.12 | 1.89 |
| 4 | 37 | 39 | 76 | 4.12 | 40.62 | 7.93 | 1.89 |
| 5 | 30 | 30 | 60 | 4.83 | 40.21 | 8.74 | 2.14 |
| 6 | 39 | 39 | 78 | 4.31 | 43.13 | 8.18 | 2.06 |
| 7 | 36 | 36 | 72 | 4.53 | 39.99 | 8.14 | 2.04 |
| 8 | 31 | 35 | 66 | 4.48 | 41.94 | 8.62 | 1.88 |
| 9 | 36 | 44 | 80 | 4.47 | 40.52 | 7.8 | 1.96 |
| 10 | 32 | 36 | 68 | 4.81 | 43.26 | 8.92 | 1.98 |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

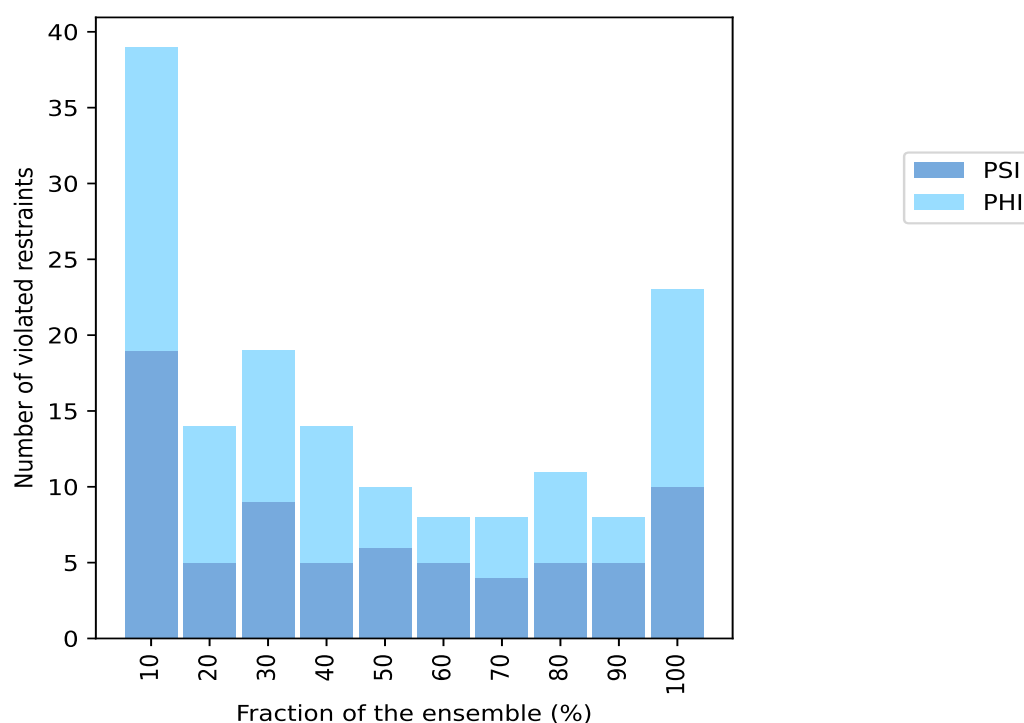
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 19 | 20 | 39 | 1 | 10.0 |
| 5 | 9 | 14 | 2 | 20.0 |
| 9 | 10 | 19 | 3 | 30.0 |
| 5 | 9 | 14 | 4 | 40.0 |
| 6 | 4 | 10 | 5 | 50.0 |
| 5 | 3 | 8 | 6 | 60.0 |
| 4 | 4 | 8 | 7 | 70.0 |
| 5 | 6 | 11 | 8 | 80.0 |
| 5 | 3 | 8 | 9 | 90.0 |
| 10 | 13 | 23 | 10 | 100.0 |

¹ Number of models with violations

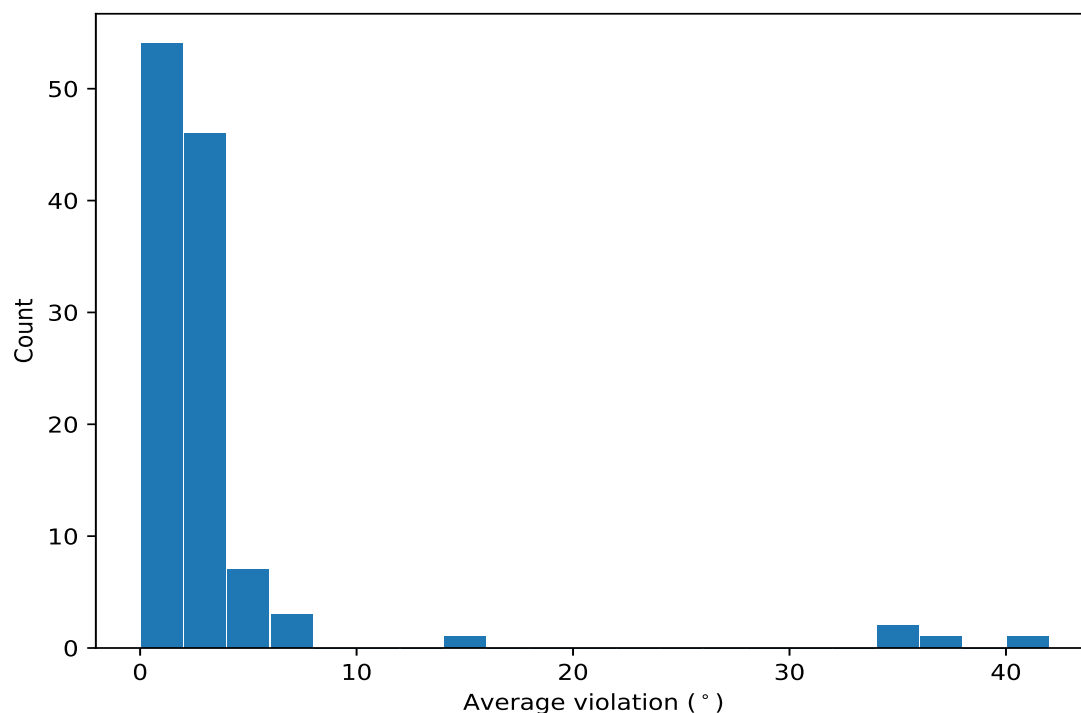
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 10 | 40.3 | 0.62 | 40.12 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 10 | 37.47 | 2.93 | 36.34 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 10 | 35.8 | 0.19 | 35.86 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 10 | 35.28 | 0.86 | 35.57 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 10 | 15.78 | 2.3 | 14.58 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 10 | 6.09 | 0.71 | 6.04 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 10 | 5.55 | 0.38 | 5.64 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 10 | 5.27 | 0.91 | 5.23 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 10 | 4.63 | 0.52 | 4.68 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 10 | 4.04 | 0.42 | 4.19 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 10 | 3.7 | 0.52 | 3.71 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 10 | 3.08 | 0.46 | 3.14 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 10 | 2.68 | 0.72 | 2.56 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 10 | 2.5 | 0.76 | 2.68 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 10 | 2.31 | 0.51 | 2.17 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 10 | 2.29 | 0.86 | 2.16 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 10 | 2.23 | 0.43 | 2.3 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 10 | 2.21 | 0.34 | 2.23 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 10 | 2.21 | 0.48 | 2.08 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 10 | 2.01 | 0.73 | 1.76 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 10 | 2.0 | 0.22 | 2.0 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 10 | 1.67 | 0.25 | 1.7 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 10 | 1.6 | 0.34 | 1.56 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 9 | 3.02 | 1.41 | 2.93 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 9 | 2.58 | 0.89 | 2.4 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 9 | 2.19 | 0.48 | 2.21 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 9 | 2.12 | 0.66 | 1.84 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 9 | 2.06 | 1.05 | 1.72 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 9 | 1.96 | 0.17 | 1.98 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 9 | 1.71 | 0.6 | 1.49 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 9 | 1.65 | 0.37 | 1.76 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 8 | 2.44 | 1.13 | 2.08 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 8 | 2.32 | 1.0 | 2.43 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 8 | 2.19 | 0.67 | 1.94 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 8 | 2.12 | 1.01 | 1.94 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 8 | 1.92 | 0.57 | 1.8 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 8 | 1.72 | 0.44 | 1.53 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 8 | 1.7 | 0.28 | 1.7 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 8 | 1.61 | 0.39 | 1.52 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 8 | 1.48 | 0.41 | 1.46 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 8 | 1.37 | 0.15 | 1.44 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 8 | 1.19 | 0.14 | 1.14 |
| (1,79) | 1:69:A:GLN:C | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 7 | 2.27 | 1.27 | 2.0 |
| (1,81) | 1:70:A:LEU:C | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 7 | 2.26 | 1.09 | 1.75 |
| (1,47) | 1:51:A:ILE:C | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C | 7 | 2.11 | 0.23 | 2.04 |
| (1,22) | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1:33:A:THR:N | 7 | 2.11 | 0.83 | 2.72 |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1:167:A:LEU:N | 7 | 1.98 | 0.89 | 1.46 |
| (1,20) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C | 1:32:A:ILE:N | 7 | 1.95 | 0.39 | 1.95 |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 7 | 1.85 | 0.22 | 1.8 |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 1:121:A:LEU:N | 7 | 1.72 | 0.58 | 1.59 |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C | 1:130:A:ASN:N | 6 | 2.38 | 0.6 | 2.53 |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N | 1:145:A:TYR:CA | 1:145:A:TYR:C | 6 | 2.09 | 0.53 | 2.36 |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 6 | 1.77 | 0.43 | 1.77 |
| (1,46) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:LYS:N | 6 | 1.61 | 0.4 | 1.48 |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 6 | 1.34 | 0.22 | 1.4 |
| (1,36) | 1:46:A:TYR:N | 1:46:A:TYR:CA | 1:46:A:TYR:C | 1:47:A:ALA:N | 6 | 1.27 | 0.16 | 1.22 |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C | 1:127:A:GLY:N | 6 | 1.25 | 0.18 | 1.27 |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C | 1:183:A:GLY:N | 6 | 1.12 | 0.09 | 1.12 |
| (1,96) | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 1:79:A:ILE:N | 5 | 4.08 | 0.31 | 4.13 |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C | 1:149:A:LYS:N | 5 | 2.44 | 0.51 | 2.38 |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N | 1:170:A:SER:CA | 1:170:A:SER:C | 5 | 2.12 | 1.09 | 1.65 |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N | 1:149:A:LYS:CA | 1:149:A:LYS:C | 5 | 2.1 | 0.49 | 1.89 |
| (1,76) | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 1:69:A:GLN:N | 5 | 2.08 | 0.74 | 1.91 |
| (1,104) | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 1:83:A:SER:N | 5 | 1.67 | 0.44 | 1.47 |

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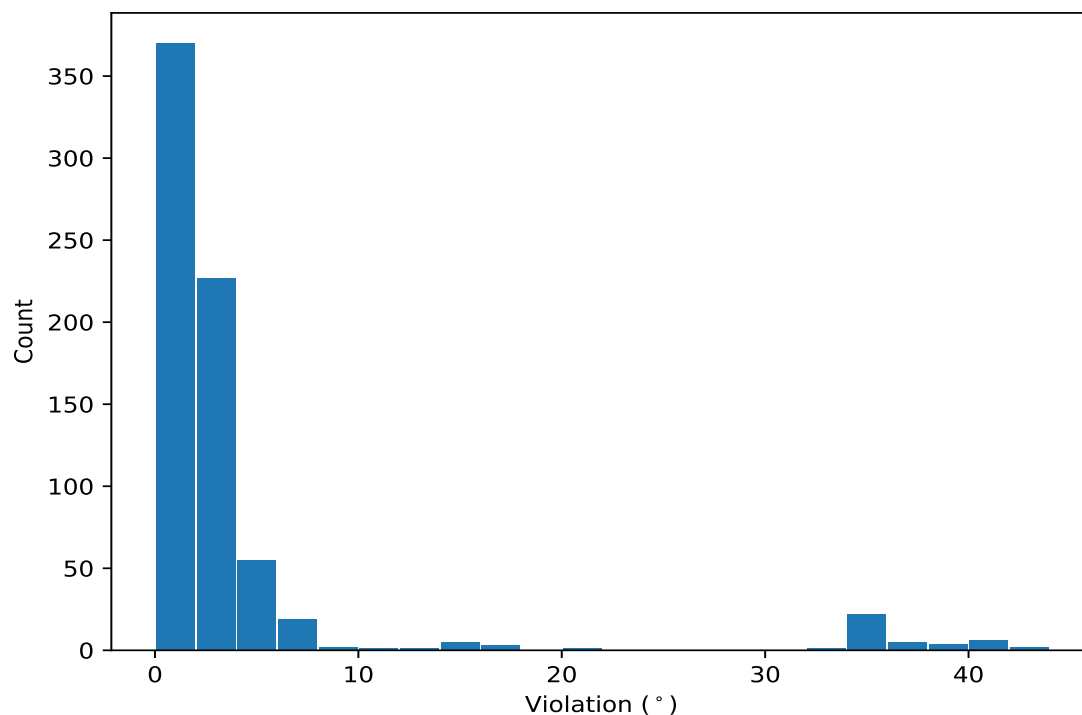
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,97) | 1:78:A:GLN:C | 1:79:A:ILE:N | 1:79:A:ILE:CA | 1:79:A:ILE:C | 5 | 1.63 | 0.19 | 1.72 |
| (1,42) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:TRP:N | 5 | 1.48 | 0.47 | 1.37 |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N | 1:171:A:LEU:CA | 1:171:A:LEU:C | 5 | 1.47 | 0.26 | 1.39 |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 1:136:A:PRO:N | 5 | 1.29 | 0.13 | 1.34 |
| (1,78) | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 1:70:A:LEU:N | 4 | 4.67 | 2.06 | 4.82 |
| (1,117) | 1:89:A:SER:C | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 4 | 3.54 | 2.08 | 3.47 |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 4 | 2.93 | 0.45 | 3.0 |
| (1,122) | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 1:93:A:GLY:N | 4 | 2.24 | 1.44 | 1.58 |
| (1,95) | 1:77:A:LEU:C | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 4 | 2.16 | 0.35 | 2.25 |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 4 | 2.09 | 0.24 | 1.98 |
| (1,106) | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 1:84:A:GLY:N | 4 | 1.88 | 0.8 | 1.56 |
| (1,85) | 1:72:A:PRO:C | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 4 | 1.87 | 0.65 | 1.66 |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 1:131:A:THR:N | 4 | 1.7 | 0.26 | 1.66 |
| (1,133) | 1:99:A:LYS:C | 1:100:A:ALA:N | 1:100:A:ALA:CA | 1:100:A:ALA:C | 4 | 1.5 | 0.32 | 1.38 |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C | 4 | 1.3 | 0.21 | 1.29 |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C | 1:138:A:GLU:N | 4 | 1.29 | 0.08 | 1.28 |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N | 1:174:A:ILE:CA | 1:174:A:ILE:C | 4 | 1.28 | 0.11 | 1.28 |
| (1,49) | 1:54:A:GLN:C | 1:55:A:VAL:N | 1:55:A:VAL:CA | 1:55:A:VAL:C | 4 | 1.24 | 0.1 | 1.24 |
| (1,121) | 1:91:A:ALA:C | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 3 | 7.19 | 4.35 | 9.99 |
| (1,120) | 1:91:A:ALA:N | 1:91:A:ALA:CA | 1:91:A:ALA:C | 1:92:A:LEU:N | 3 | 6.09 | 2.63 | 7.49 |
| (1,116) | 1:89:A:SER:N | 1:89:A:SER:CA | 1:89:A:SER:C | 1:90:A:THR:N | 3 | 5.68 | 3.03 | 7.67 |
| (1,124) | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 1:96:A:SER:N | 3 | 3.87 | 0.45 | 3.65 |
| (1,44) | 1:50:A:TRP:N | 1:50:A:TRP:CA | 1:50:A:TRP:C | 1:51:A:ILE:N | 3 | 3.81 | 0.25 | 3.77 |
| (1,45) | 1:50:A:TRP:C | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 3 | 3.37 | 0.23 | 3.48 |
| (1,125) | 1:95:A:PHE:C | 1:96:A:SER:N | 1:96:A:SER:CA | 1:96:A:SER:C | 3 | 3.25 | 0.39 | 3.13 |
| (1,92) | 1:76:A:TYR:N | 1:76:A:TYR:CA | 1:76:A:TYR:C | 1:77:A:LEU:N | 3 | 2.44 | 1.57 | 1.6 |
| (1,241) | 1:159:A:PHE:C | 1:160:A:TYR:N | 1:160:A:TYR:CA | 1:160:A:TYR:C | 3 | 2.31 | 0.19 | 2.18 |
| (1,86) | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 1:74:A:PHE:N | 3 | 2.04 | 0.61 | 1.98 |
| (1,25) | 1:33:A:THR:C | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 3 | 1.89 | 0.54 | 1.76 |
| (1,131) | 1:98:A:THR:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 3 | 1.73 | 0.38 | 1.88 |
| (1,189) | 1:130:A:ASN:C | 1:131:A:THR:N | 1:131:A:THR:CA | 1:131:A:THR:C | 3 | 1.55 | 0.28 | 1.45 |
| (1,184) | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 1:128:A:TYR:N | 3 | 1.53 | 0.14 | 1.51 |
| (1,126) | 1:96:A:SER:N | 1:96:A:SER:CA | 1:96:A:SER:C | 1:97:A:GLU:N | 3 | 1.51 | 0.04 | 1.5 |
| (1,212) | 1:144:A:VAL:N | 1:144:A:VAL:CA | 1:144:A:VAL:C | 1:145:A:TYR:N | 3 | 1.5 | 0.3 | 1.63 |
| (1,3) | 1:22:A:PRO:C | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C | 3 | 1.48 | 0.35 | 1.35 |
| (1,169) | 1:118:A:ILE:C | 1:119:A:ALA:N | 1:119:A:ALA:CA | 1:119:A:ALA:C | 3 | 1.4 | 0.4 | 1.22 |
| (1,73) | 1:66:A:ASN:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 3 | 1.22 | 0.15 | 1.17 |
| (1,113) | 1:86:A:GLU:C | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 2 | 3.26 | 1.36 | 3.26 |
| (1,252) | 1:165:A:GLY:N | 1:165:A:GLY:CA | 1:165:A:GLY:C | 1:166:A:MET:N | 2 | 2.58 | 0.17 | 2.58 |
| (1,111) | 1:85:A:TYR:C | 1:86:A:GLU:N | 1:86:A:GLU:CA | 1:86:A:GLU:C | 2 | 2.46 | 0.96 | 2.46 |
| (1,107) | 1:83:A:SER:C | 1:84:A:GLY:N | 1:84:A:GLY:CA | 1:84:A:GLY:C | 2 | 2.22 | 0.84 | 2.22 |
| (1,87) | 1:73:A:TYR:C | 1:74:A:PHE:N | 1:74:A:PHE:CA | 1:74:A:PHE:C | 2 | 1.73 | 0.71 | 1.73 |
| (1,177) | 1:122:A:TYR:C | 1:123:A:PRO:N | 1:123:A:PRO:CA | 1:123:A:PRO:C | 2 | 1.5 | 0.4 | 1.5 |
| (1,118) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:ALA:N | 2 | 1.46 | 0.29 | 1.46 |
| (1,84) | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 1:73:A:TYR:N | 2 | 1.45 | 0.24 | 1.45 |
| (1,148) | 1:108:A:SER:N | 1:108:A:SER:CA | 1:108:A:SER:C | 1:109:A:ALA:N | 2 | 1.32 | 0.21 | 1.32 |
| (1,173) | 1:120:A:VAL:C | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C | 2 | 1.3 | 0.15 | 1.3 |
| (1,215) | 1:146:A:ASN:C | 1:147:A:GLU:N | 1:147:A:GLU:CA | 1:147:A:GLU:C | 2 | 1.3 | 0.08 | 1.3 |
| (1,146) | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 1:107:A:PRO:N | 2 | 1.18 | 0.16 | 1.18 |
| (1,195) | 1:133:A:ILE:C | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 2 | 1.11 | 0.06 | 1.11 |
| (1,119) | 1:90:A:THR:C | 1:91:A:ALA:N | 1:91:A:ALA:CA | 1:91:A:ALA:C | 2 | 1.06 | 0.06 | 1.06 |

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 10 | 43.26 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 6 | 43.13 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 8 | 41.94 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 4 | 40.62 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 9 | 40.52 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 3 | 40.34 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 5 | 40.21 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 1 | 40.03 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 7 | 39.99 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 2 | 39.91 |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 10 | 39.81 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 6 | 39.66 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 3 | 37.22 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 8 | 36.78 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 2 | 36.68 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 2 | 36.14 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 4 | 36.0 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 7 | 35.94 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 10 | 35.94 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 5 | 35.91 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 8 | 35.91 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 7 | 35.86 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 9 | 35.86 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 6 | 35.84 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 4 | 35.75 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 3 | 35.72 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 10 | 35.67 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 8 | 35.61 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 6 | 35.61 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 1 | 35.54 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 4 | 35.53 |
| (1,14) | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1:29:A:LEU:N | 3 | 35.51 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 9 | 35.48 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 7 | 35.46 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 1 | 35.36 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 9 | 35.33 |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 5 | 35.31 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 2 | 35.27 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 5 | 35.11 |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N | 1:113:A:LEU:CA | 1:113:A:LEU:C | 1 | 32.8 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 10 | 21.35 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 3 | 17.55 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 7 | 17.31 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 9 | 16.44 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 5 | 14.64 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 6 | 14.52 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 2 | 14.31 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 8 | 14.13 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 1 | 14.1 |
| (1,9) | 1:25:A:VAL:C | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 4 | 13.45 |
| (1,121) | 1:91:A:ALA:C | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 9 | 10.53 |
| (1,121) | 1:91:A:ALA:C | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 2 | 9.99 |
| (1,120) | 1:91:A:ALA:N | 1:91:A:ALA:CA | 1:91:A:ALA:C | 1:92:A:LEU:N | 2 | 8.38 |
| (1,116) | 1:89:A:SER:N | 1:89:A:SER:CA | 1:89:A:SER:C | 1:90:A:THR:N | 9 | 7.98 |
| (1,116) | 1:89:A:SER:N | 1:89:A:SER:CA | 1:89:A:SER:C | 1:90:A:THR:N | 2 | 7.67 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 7 | 7.66 |
| (1,120) | 1:91:A:ALA:N | 1:91:A:ALA:CA | 1:91:A:ALA:C | 1:92:A:LEU:N | 9 | 7.49 |
| (1,5) | 1:23:A:ILE:C | 1:24:A:ASP:N | 1:24:A:ASP:CA | 1:24:A:ASP:C | 10 | 7.44 |
| (1,78) | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 1:70:A:LEU:N | 9 | 7.04 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 10 | 6.85 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 1 | 6.81 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 10 | 6.56 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 9 | 6.32 |
| (1,78) | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 1:70:A:LEU:N | 10 | 6.28 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 5 | 6.26 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 6 | 6.22 |
| (1,117) | 1:89:A:SER:C | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 9 | 6.2 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 7 | 6.05 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 8 | 6.05 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 4 | 6.04 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 3 | 6.03 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 10 | 6.01 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 8 | 5.88 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 1 | 5.87 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 4 | 5.78 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 8 | 5.73 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 5 | 5.72 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 9 | 5.64 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 10 | 5.63 |
| (1,200) | 1:136:A:PRO:N | 1:136:A:PRO:CA | 1:136:A:PRO:C | 1:137:A:GLY:N | 7 | 5.56 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 2 | 5.56 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 3 | 5.55 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 6 | 5.31 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 3 | 5.21 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 1 | 5.13 |
| (1,79) | 1:69:A:GLN:C | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 9 | 5.11 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 2 | 5.1 |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 1:135:A:VAL:N | 9 | 5.09 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 3 | 5.05 |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1:139:A:PRO:N | 5 | 4.96 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 6 | 4.93 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 6 | 4.91 |
| (1,117) | 1:89:A:SER:C | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 2 | 4.86 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 4 | 4.85 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 7 | 4.84 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 5 | 4.79 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 3 | 4.75 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 5 | 4.71 |
| (1,122) | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 1:93:A:GLY:N | 7 | 4.7 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 8 | 4.66 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 1 | 4.64 |
| (1,92) | 1:76:A:TYR:N | 1:76:A:TYR:CA | 1:76:A:TYR:C | 1:77:A:LEU:N | 10 | 4.64 |
| (1,113) | 1:86:A:GLU:C | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 9 | 4.61 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 7 | 4.61 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 5 | 4.57 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 4 | 4.51 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1 | 4.51 |
| (1,124) | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 1:96:A:SER:N | 7 | 4.5 |
| (1,81) | 1:70:A:LEU:C | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 8 | 4.48 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 6 | 4.44 |
| (1,96) | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 1:79:A:ILE:N | 9 | 4.44 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 3 | 4.39 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 10 | 4.38 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,96) | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 1:79:A:ILE:N | 6 | 4.37 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 7 | 4.36 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 9 | 4.33 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 9 | 4.3 |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N | 1:170:A:SER:CA | 1:170:A:SER:C | 2 | 4.27 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 1 | 4.23 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 8 | 4.21 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 1 | 4.17 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 2 | 4.17 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 2 | 4.14 |
| (1,96) | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 1:79:A:ILE:N | 1 | 4.13 |
| (1,44) | 1:50:A:TRP:N | 1:50:A:TRP:CA | 1:50:A:TRP:C | 1:51:A:ILE:N | 7 | 4.13 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 3 | 4.06 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 4 | 4.02 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 7 | 3.99 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 2 | 3.98 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 3 | 3.98 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 6 | 3.91 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 9 | 3.9 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 2 | 3.87 |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N | 1:151:A:VAL:CA | 1:151:A:VAL:C | 2 | 3.87 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 10 | 3.81 |
| (1,96) | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 1:79:A:ILE:N | 5 | 3.8 |
| (1,125) | 1:95:A:PHE:C | 1:96:A:SER:N | 1:96:A:SER:CA | 1:96:A:SER:C | 7 | 3.77 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 3 | 3.77 |
| (1,44) | 1:50:A:TRP:N | 1:50:A:TRP:CA | 1:50:A:TRP:C | 1:51:A:ILE:N | 4 | 3.77 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 5 | 3.75 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 7 | 3.72 |
| (1,24) | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 1:34:A:PRO:N | 2 | 3.68 |
| (1,96) | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 1:79:A:ILE:N | 2 | 3.66 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 10 | 3.66 |
| (1,124) | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 1:96:A:SER:N | 6 | 3.65 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 7 | 3.63 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 5 | 3.61 |
| (1,45) | 1:50:A:TRP:C | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 7 | 3.59 |
| (1,44) | 1:50:A:TRP:N | 1:50:A:TRP:CA | 1:50:A:TRP:C | 1:51:A:ILE:N | 6 | 3.52 |
| (1,45) | 1:50:A:TRP:C | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 4 | 3.48 |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 4 | 3.47 |
| (1,124) | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 1:96:A:SER:N | 3 | 3.47 |
| (1,76) | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 1:69:A:GLN:N | 5 | 3.45 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 4 | 3.45 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 9 | 3.44 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 8 | 3.43 |
| (1,111) | 1:85:A:TYR:C | 1:86:A:GLU:N | 1:86:A:GLU:CA | 1:86:A:GLU:C | 2 | 3.41 |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C | 1:149:A:LYS:N | 4 | 3.37 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 10 | 3.36 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 1 | 3.35 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 3 | 3.35 |
| (1,78) | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 1:70:A:LEU:N | 8 | 3.35 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 9 | 3.29 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 7 | 3.28 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 6 | 3.27 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 1 | 3.27 |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1:167:A:LEU:N | 6 | 3.25 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 2 | 3.23 |
| (1,81) | 1:70:A:LEU:C | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 6 | 3.23 |
| (1,106) | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 1:84:A:GLY:N | 2 | 3.19 |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1:167:A:LEU:N | 8 | 3.18 |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1 | 3.17 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 6 | 3.17 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 7 | 3.16 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 5 | 3.16 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 1 | 3.13 |
| (1,125) | 1:95:A:PHE:C | 1:96:A:SER:N | 1:96:A:SER:CA | 1:96:A:SER:C | 6 | 3.13 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 9 | 3.11 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 1 | 3.1 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 2 | 3.1 |
| (1,80) | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 1:71:A:LYS:N | 8 | 3.09 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 6 | 3.09 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 6 | 3.08 |
| (1,107) | 1:83:A:SER:C | 1:84:A:GLY:N | 1:84:A:GLY:CA | 1:84:A:GLY:C | 2 | 3.05 |
| (1,45) | 1:50:A:TRP:C | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 6 | 3.05 |
| (1,7) | 1:24:A:ASP:C | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 6 | 3.04 |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N | 1:149:A:LYS:CA | 1:149:A:LYS:C | 4 | 3.02 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 4 | 3.02 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 7 | 3.01 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 6 | 2.97 |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C | 1:130:A:ASN:N | 6 | 2.95 |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C | 1:130:A:ASN:N | 9 | 2.94 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 9 | 2.93 |
| (1,85) | 1:72:A:PRO:C | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 10 | 2.92 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 10 | 2.92 |
| (1,22) | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1:33:A:THR:N | 5 | 2.9 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 4 | 2.87 |
| (1,125) | 1:95:A:PHE:C | 1:96:A:SER:N | 1:96:A:SER:CA | 1:96:A:SER:C | 3 | 2.85 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 10 | 2.85 |
| (1,22) | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1:33:A:THR:N | 6 | 2.85 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 4 | 2.84 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 10 | 2.84 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 9 | 2.83 |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 10 | 2.82 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 3 | 2.82 |
| (1,12) | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1:28:A:HIS:N | 2 | 2.82 |
| (1,86) | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 1:74:A:PHE:N | 6 | 2.81 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 8 | 2.81 |
| (1,22) | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1:33:A:THR:N | 1 | 2.8 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 3 | 2.77 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 3 | 2.77 |
| (1,252) | 1:165:A:GLY:N | 1:165:A:GLY:CA | 1:165:A:GLY:C | 1:166:A:MET:N | 10 | 2.75 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 4 | 2.74 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 2 | 2.73 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 5 | 2.72 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,22) | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1:33:A:THR:N | 9 | 2.72 |
| (1,77) | 1:68:A:GLU:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 8 | 2.71 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 7 | 2.7 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 8 | 2.7 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 6 | 2.69 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 9 | 2.67 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 5 | 2.65 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 7 | 2.64 |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C | 1:130:A:ASN:N | 4 | 2.64 |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 1:121:A:LEU:N | 4 | 2.64 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 2 | 2.62 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 3 | 2.62 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 5 | 2.62 |
| (1,25) | 1:33:A:THR:C | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 10 | 2.6 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 1 | 2.59 |
| (1,241) | 1:159:A:PHE:C | 1:160:A:TYR:N | 1:160:A:TYR:CA | 1:160:A:TYR:C | 1 | 2.58 |
| (1,20) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C | 1:32:A:ILE:N | 8 | 2.58 |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N | 1:145:A:TYR:CA | 1:145:A:TYR:C | 9 | 2.57 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 5 | 2.56 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 6 | 2.56 |
| (1,95) | 1:77:A:LEU:C | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 4 | 2.54 |
| (1,79) | 1:69:A:GLN:C | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 7 | 2.52 |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N | 1:145:A:TYR:CA | 1:145:A:TYR:C | 4 | 2.51 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 3 | 2.51 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 2 | 2.51 |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1:167:A:LEU:N | 7 | 2.5 |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C | 1:149:A:LYS:N | 5 | 2.5 |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 9 | 2.5 |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 1:121:A:LEU:N | 6 | 2.5 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 8 | 2.49 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 7 | 2.48 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 6 | 2.47 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 6 | 2.47 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 5 | 2.47 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 10 | 2.45 |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N | 1:145:A:TYR:CA | 1:145:A:TYR:C | 10 | 2.44 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 7 | 2.44 |
| (1,87) | 1:73:A:TYR:C | 1:74:A:PHE:N | 1:74:A:PHE:CA | 1:74:A:PHE:C | 2 | 2.44 |
| (1,252) | 1:165:A:GLY:N | 1:165:A:GLY:CA | 1:165:A:GLY:C | 1:166:A:MET:N | 4 | 2.42 |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C | 1:130:A:ASN:N | 1 | 2.42 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 4 | 2.42 |
| (1,20) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C | 1:32:A:ILE:N | 5 | 2.42 |
| (1,120) | 1:91:A:ALA:N | 1:91:A:ALA:CA | 1:91:A:ALA:C | 1:92:A:LEU:N | 10 | 2.4 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 6 | 2.4 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 5 | 2.4 |
| (1,13) | 1:27:A:SER:C | 1:28:A:HIS:N | 1:28:A:HIS:CA | 1:28:A:HIS:C | 2 | 2.4 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 6 | 2.39 |
| (1,47) | 1:51:A:ILE:C | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C | 5 | 2.39 |
| (1,42) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:TRP:N | 5 | 2.39 |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C | 1:149:A:LYS:N | 3 | 2.38 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 7 | 2.38 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 6 | 2.38 |
| (1,47) | 1:51:A:ILE:C | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C | 8 | 2.37 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 9 | 2.37 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 7 | 2.36 |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 10 | 2.34 |
| (1,47) | 1:51:A:ILE:C | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C | 10 | 2.34 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 10 | 2.34 |
| (1,95) | 1:77:A:LEU:C | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 10 | 2.33 |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 2 | 2.32 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 3 | 2.31 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 2 | 2.31 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 3 | 2.3 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 2 | 2.3 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 8 | 2.29 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 1 | 2.29 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 4 | 2.29 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 7 | 2.29 |
| (1,104) | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 1:83:A:SER:N | 2 | 2.28 |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 9 | 2.27 |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N | 1:145:A:TYR:CA | 1:145:A:TYR:C | 5 | 2.27 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 3 | 2.27 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 6 | 2.26 |
| (1,79) | 1:69:A:GLN:C | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 2 | 2.26 |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 4 | 2.25 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 8 | 2.25 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 1 | 2.25 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 2 | 2.24 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 5 | 2.23 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 7 | 2.22 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 10 | 2.21 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 2 | 2.21 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 4 | 2.21 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 1 | 2.2 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 3 | 2.2 |
| (1,46) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:LYS:N | 7 | 2.2 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 6 | 2.19 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 8 | 2.19 |
| (1,241) | 1:159:A:PHE:C | 1:160:A:TYR:N | 1:160:A:TYR:CA | 1:160:A:TYR:C | 2 | 2.18 |
| (1,76) | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 1:69:A:GLN:N | 3 | 2.18 |
| (1,264) | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 1:173:A:VAL:N | 9 | 2.17 |
| (1,241) | 1:159:A:PHE:C | 1:160:A:TYR:N | 1:160:A:TYR:CA | 1:160:A:TYR:C | 6 | 2.17 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 1 | 2.17 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 8 | 2.17 |
| (1,112) | 1:86:A:GLU:N | 1:86:A:GLU:CA | 1:86:A:GLU:C | 1:87:A:THR:N | 9 | 2.17 |
| (1,95) | 1:77:A:LEU:C | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 8 | 2.17 |
| (1,23) | 1:32:A:ILE:C | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C | 2 | 2.17 |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N | 1:149:A:LYS:CA | 1:149:A:LYS:C | 5 | 2.16 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 7 | 2.16 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 1 | 2.16 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 9 | 2.16 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 2 | 2.15 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 2 | 2.14 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 2 | 2.13 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 9 | 2.12 |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 1:131:A:THR:N | 6 | 2.12 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 2 | 2.12 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 4 | 2.12 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 5 | 2.12 |
| (1,262) | 1:171:A:LEU:N | 1:171:A:LEU:CA | 1:171:A:LEU:C | 1:172:A:PRO:N | 2 | 2.11 |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C | 1:130:A:ASN:N | 3 | 2.11 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 3 | 2.11 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 9 | 2.11 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 8 | 2.1 |
| (1,131) | 1:98:A:THR:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 8 | 2.1 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 3 | 2.1 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 4 | 2.09 |
| (1,104) | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 1:83:A:SER:N | 9 | 2.09 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 4 | 2.09 |
| (1,117) | 1:89:A:SER:C | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 10 | 2.08 |
| (1,46) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:LYS:N | 4 | 2.08 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 7 | 2.07 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 1 | 2.06 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 4 | 2.06 |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C | 1:149:A:LYS:N | 1 | 2.05 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 9 | 2.05 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 1 | 2.05 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 1 | 2.04 |
| (1,133) | 1:99:A:LYS:C | 1:100:A:ALA:N | 1:100:A:ALA:CA | 1:100:A:ALA:C | 7 | 2.04 |
| (1,47) | 1:51:A:ILE:C | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C | 3 | 2.04 |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 4 | 2.03 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 7 | 2.03 |
| (1,227) | 1:152:A:ALA:C | 1:153:A:ILE:N | 1:153:A:ILE:CA | 1:153:A:ILE:C | 2 | 2.02 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 5 | 2.02 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 8 | 2.02 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 9 | 2.01 |
| (1,78) | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 1:70:A:LEU:N | 6 | 2.01 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 2 | 2.01 |
| (1,79) | 1:69:A:GLN:C | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 10 | 2.0 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 10 | 1.99 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 7 | 1.98 |
| (1,86) | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 1:74:A:PHE:N | 2 | 1.98 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 5 | 1.97 |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N | 1:171:A:LEU:CA | 1:171:A:LEU:C | 9 | 1.96 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 3 | 1.96 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 10 | 1.96 |
| (1,169) | 1:118:A:ILE:C | 1:119:A:ALA:N | 1:119:A:ALA:CA | 1:119:A:ALA:C | 6 | 1.96 |
| (1,47) | 1:51:A:ILE:C | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C | 9 | 1.96 |
| (1,20) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C | 1:32:A:ILE:N | 2 | 1.96 |
| (1,3) | 1:22:A:PRO:C | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C | 3 | 1.96 |
| (1,20) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C | 1:32:A:ILE:N | 9 | 1.95 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 2 | 1.94 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 5 | 1.94 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 4 | 1.94 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 7 | 1.94 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 8 | 1.93 |
| (1,189) | 1:130:A:ASN:C | 1:131:A:THR:N | 1:131:A:THR:CA | 1:131:A:THR:C | 6 | 1.93 |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 3 | 1.93 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 1 | 1.93 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 5 | 1.93 |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C | 1:149:A:LYS:N | 7 | 1.92 |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 1 | 1.92 |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C | 1:123:A:PRO:N | 7 | 1.92 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 6 | 1.92 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 7 | 1.91 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 2 | 1.91 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 3 | 1.91 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 4 | 1.91 |
| (1,177) | 1:122:A:TYR:C | 1:123:A:PRO:N | 1:123:A:PRO:CA | 1:123:A:PRO:C | 2 | 1.91 |
| (1,85) | 1:72:A:PRO:C | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 8 | 1.91 |
| (1,76) | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 1:69:A:GLN:N | 6 | 1.91 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 6 | 1.91 |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N | 1:170:A:SER:CA | 1:170:A:SER:C | 8 | 1.9 |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 5 | 1.9 |
| (1,113) | 1:86:A:GLU:C | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 2 | 1.9 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 7 | 1.9 |
| (1,79) | 1:69:A:GLN:C | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 1 | 1.9 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 4 | 1.9 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 8 | 1.89 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 9 | 1.89 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 3 | 1.89 |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N | 1:149:A:LYS:CA | 1:149:A:LYS:C | 3 | 1.89 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 9 | 1.89 |
| (1,131) | 1:98:A:THR:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 4 | 1.88 |
| (1,106) | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 1:84:A:GLY:N | 3 | 1.88 |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 4 | 1.87 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 9 | 1.87 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 5 | 1.86 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 6 | 1.86 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 8 | 1.86 |
| (1,81) | 1:70:A:LEU:C | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 2 | 1.86 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 2 | 1.85 |
| (1,47) | 1:51:A:ILE:C | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C | 1 | 1.85 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 10 | 1.84 |
| (1,97) | 1:78:A:GLN:C | 1:79:A:ILE:N | 1:79:A:ILE:CA | 1:79:A:ILE:C | 4 | 1.84 |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 5 | 1.83 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 7 | 1.83 |
| (1,47) | 1:51:A:ILE:C | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C | 2 | 1.83 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 4 | 1.81 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 7 | 1.81 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 8 | 1.81 |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 2 | 1.8 |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 3 | 1.8 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 2 | 1.8 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N | 1:149:A:LYS:CA | 1:149:A:LYS:C | 7 | 1.8 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 9 | 1.79 |
| (1,212) | 1:144:A:VAL:N | 1:144:A:VAL:CA | 1:144:A:VAL:C | 1:145:A:TYR:N | 10 | 1.79 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 1 | 1.78 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 7 | 1.78 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 2 | 1.78 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 6 | 1.77 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 8 | 1.77 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 1 | 1.76 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 5 | 1.76 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 6 | 1.76 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 10 | 1.76 |
| (1,25) | 1:33:A:THR:C | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 2 | 1.76 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 4 | 1.75 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 3 | 1.75 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 5 | 1.75 |
| (1,118) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:ALA:N | 9 | 1.75 |
| (1,81) | 1:70:A:LEU:C | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1 | 1.75 |
| (1,81) | 1:70:A:LEU:C | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 7 | 1.75 |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 8 | 1.74 |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N | 1:158:A:ALA:CA | 1:158:A:ALA:C | 10 | 1.74 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 9 | 1.74 |
| (1,97) | 1:78:A:GLN:C | 1:79:A:ILE:N | 1:79:A:ILE:CA | 1:79:A:ILE:C | 8 | 1.74 |
| (1,122) | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 1:93:A:GLY:N | 10 | 1.73 |
| (1,97) | 1:78:A:GLN:C | 1:79:A:ILE:N | 1:79:A:ILE:CA | 1:79:A:ILE:C | 10 | 1.72 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 8 | 1.72 |
| (1,217) | 1:147:A:GLU:C | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C | 8 | 1.71 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 2 | 1.71 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 7 | 1.71 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 10 | 1.7 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 8 | 1.7 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 9 | 1.7 |
| (1,184) | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 1:128:A:TYR:N | 3 | 1.7 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 9 | 1.69 |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 1:131:A:THR:N | 4 | 1.69 |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 1:121:A:LEU:N | 3 | 1.69 |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C | 1:106:A:ASN:N | 10 | 1.69 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 10 | 1.69 |
| (1,84) | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 1:73:A:TYR:N | 6 | 1.69 |
| (1,20) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C | 1:32:A:ILE:N | 6 | 1.69 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 6 | 1.68 |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N | 1:164:A:GLU:CA | 1:164:A:GLU:C | 9 | 1.67 |
| (1,81) | 1:70:A:LEU:C | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 9 | 1.67 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 3 | 1.66 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 6 | 1.66 |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N | 1:170:A:SER:CA | 1:170:A:SER:C | 4 | 1.65 |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N | 1:149:A:LYS:CA | 1:149:A:LYS:C | 1 | 1.65 |
| (1,59) | 1:59:A:LYS:C | 1:60:A:LEU:N | 1:60:A:LEU:CA | 1:60:A:LEU:C | 3 | 1.65 |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 7 | 1.64 |
| (1,212) | 1:144:A:VAL:N | 1:144:A:VAL:CA | 1:144:A:VAL:C | 1:145:A:TYR:N | 4 | 1.63 |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 1:131:A:THR:N | 1 | 1.62 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,46) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:LYS:N | 6 | 1.62 |
| (1,258) | 1:168:A:PHE:N | 1:168:A:PHE:CA | 1:168:A:PHE:C | 1:169:A:ASP:N | 2 | 1.61 |
| (1,161) | 1:114:A:ASP:C | 1:115:A:LYS:N | 1:115:A:LYS:CA | 1:115:A:LYS:C | 9 | 1.61 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 1 | 1.61 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 9 | 1.61 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 10 | 1.61 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 3 | 1.6 |
| (1,92) | 1:76:A:TYR:N | 1:76:A:TYR:CA | 1:76:A:TYR:C | 1:77:A:LEU:N | 2 | 1.6 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 3 | 1.6 |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C | 9 | 1.59 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 6 | 1.59 |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 8 | 1.59 |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 1:121:A:LEU:N | 9 | 1.59 |
| (1,95) | 1:77:A:LEU:C | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 7 | 1.59 |
| (1,26) | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 1:35:A:ALA:N | 10 | 1.59 |
| (1,20) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C | 1:32:A:ILE:N | 1 | 1.59 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 6 | 1.58 |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C | 4 | 1.58 |
| (1,127) | 1:96:A:SER:C | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 8 | 1.58 |
| (1,74) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 1:68:A:GLU:N | 4 | 1.58 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 4 | 1.57 |
| (1,147) | 1:107:A:PRO:C | 1:108:A:SER:N | 1:108:A:SER:CA | 1:108:A:SER:C | 7 | 1.56 |
| (1,126) | 1:96:A:SER:N | 1:96:A:SER:CA | 1:96:A:SER:C | 1:97:A:GLU:N | 9 | 1.56 |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N | 1:145:A:TYR:CA | 1:145:A:TYR:C | 8 | 1.55 |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 4 | 1.55 |
| (1,128) | 1:97:A:GLU:N | 1:97:A:GLU:CA | 1:97:A:GLU:C | 1:98:A:THR:N | 7 | 1.55 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 3 | 1.54 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 10 | 1.54 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 8 | 1.54 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 6 | 1.53 |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C | 1:127:A:GLY:N | 8 | 1.53 |
| (1,148) | 1:108:A:SER:N | 1:108:A:SER:CA | 1:108:A:SER:C | 1:109:A:ALA:N | 6 | 1.53 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 8 | 1.52 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 10 | 1.52 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 5 | 1.52 |
| (1,97) | 1:78:A:GLN:C | 1:79:A:ILE:N | 1:79:A:ILE:CA | 1:79:A:ILE:C | 7 | 1.52 |
| (1,184) | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 1:128:A:TYR:N | 4 | 1.51 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 3 | 1.51 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 4 | 1.51 |
| (1,36) | 1:46:A:TYR:N | 1:46:A:TYR:CA | 1:46:A:TYR:C | 1:47:A:ALA:N | 6 | 1.51 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 5 | 1.5 |
| (1,126) | 1:96:A:SER:N | 1:96:A:SER:CA | 1:96:A:SER:C | 1:97:A:GLU:N | 2 | 1.5 |
| (1,115) | 1:88:A:ASN:C | 1:89:A:SER:N | 1:89:A:SER:CA | 1:89:A:SER:C | 9 | 1.5 |
| (1,111) | 1:85:A:TYR:C | 1:86:A:GLU:N | 1:86:A:GLU:CA | 1:86:A:GLU:C | 9 | 1.5 |
| (1,76) | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 1:69:A:GLN:N | 7 | 1.49 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 3 | 1.49 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 5 | 1.49 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 5 | 1.48 |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 3 | 1.48 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 9 | 1.48 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 7 | 1.47 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 1 | 1.47 |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 1:121:A:LEU:N | 1 | 1.47 |
| (1,104) | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 1:83:A:SER:N | 3 | 1.47 |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N | 1:170:A:SER:CA | 1:170:A:SER:C | 5 | 1.46 |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1:167:A:LEU:N | 4 | 1.46 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 6 | 1.46 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 8 | 1.46 |
| (1,133) | 1:99:A:LYS:C | 1:100:A:ALA:N | 1:100:A:ALA:CA | 1:100:A:ALA:C | 6 | 1.46 |
| (1,126) | 1:96:A:SER:N | 1:96:A:SER:CA | 1:96:A:SER:C | 1:97:A:GLU:N | 5 | 1.46 |
| (1,36) | 1:46:A:TYR:N | 1:46:A:TYR:CA | 1:46:A:TYR:C | 1:47:A:ALA:N | 4 | 1.46 |
| (1,20) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C | 1:32:A:ILE:N | 7 | 1.46 |
| (1,189) | 1:130:A:ASN:C | 1:131:A:THR:N | 1:131:A:THR:CA | 1:131:A:THR:C | 4 | 1.45 |
| (1,173) | 1:120:A:VAL:C | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C | 4 | 1.45 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 10 | 1.45 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 7 | 1.45 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 5 | 1.44 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 1 | 1.44 |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N | 1:174:A:ILE:CA | 1:174:A:ILE:C | 6 | 1.43 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 3 | 1.43 |
| (1,122) | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 1:93:A:GLY:N | 8 | 1.43 |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N | 1:171:A:LEU:CA | 1:171:A:LEU:C | 2 | 1.42 |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C | 1:142:A:ILE:N | 8 | 1.42 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 4 | 1.42 |
| (1,73) | 1:66:A:ASN:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 6 | 1.42 |
| (1,260) | 1:170:A:SER:N | 1:170:A:SER:CA | 1:170:A:SER:C | 1:171:A:LEU:N | 2 | 1.41 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 1 | 1.41 |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C | 1:164:A:GLU:N | 5 | 1.41 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 9 | 1.41 |
| (1,85) | 1:72:A:PRO:C | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 9 | 1.41 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 2 | 1.4 |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C | 1:138:A:GLU:N | 8 | 1.4 |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 1:136:A:PRO:N | 6 | 1.4 |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C | 5 | 1.4 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 2 | 1.4 |
| (1,116) | 1:89:A:SER:N | 1:89:A:SER:CA | 1:89:A:SER:C | 1:90:A:THR:N | 10 | 1.4 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 9 | 1.4 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 9 | 1.4 |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N | 1:171:A:LEU:CA | 1:171:A:LEU:C | 6 | 1.39 |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C | 1:131:A:THR:N | 9 | 1.39 |
| (1,93) | 1:76:A:TYR:C | 1:77:A:LEU:N | 1:77:A:LEU:CA | 1:77:A:LEU:C | 3 | 1.39 |
| (1,76) | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 1:69:A:GLN:N | 4 | 1.39 |
| (1,62) | 1:61:A:LYS:N | 1:61:A:LYS:CA | 1:61:A:LYS:C | 1:62:A:VAL:N | 4 | 1.39 |
| (1,42) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:TRP:N | 8 | 1.39 |
| (1,215) | 1:146:A:ASN:C | 1:147:A:GLU:N | 1:147:A:GLU:CA | 1:147:A:GLU:C | 10 | 1.38 |
| (1,138) | 1:102:A:ILE:N | 1:102:A:ILE:CA | 1:102:A:ILE:C | 1:103:A:SER:N | 1 | 1.38 |
| (1,107) | 1:83:A:SER:C | 1:84:A:GLY:N | 1:84:A:GLY:CA | 1:84:A:GLY:C | 3 | 1.38 |
| (1,49) | 1:54:A:GLN:C | 1:55:A:VAL:N | 1:55:A:VAL:CA | 1:55:A:VAL:C | 4 | 1.38 |
| (1,184) | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 1:128:A:TYR:N | 1 | 1.37 |
| (1,42) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:TRP:N | 4 | 1.37 |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N | 1:171:A:LEU:CA | 1:171:A:LEU:C | 1 | 1.36 |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 1:136:A:PRO:N | 7 | 1.35 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C | 1:127:A:GLY:N | 1 | 1.35 |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C | 1:127:A:GLY:N | 4 | 1.35 |
| (1,180) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C | 1:125:A:LYS:N | 2 | 1.35 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 5 | 1.35 |
| (1,46) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:LYS:N | 5 | 1.35 |
| (1,3) | 1:22:A:PRO:C | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C | 4 | 1.35 |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N | 1:174:A:ILE:CA | 1:174:A:ILE:C | 1 | 1.34 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 9 | 1.34 |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 1:136:A:PRO:N | 1 | 1.34 |
| (1,146) | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 1:107:A:PRO:N | 2 | 1.34 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 8 | 1.34 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 8 | 1.34 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 8 | 1.34 |
| (1,86) | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 1:74:A:PHE:N | 8 | 1.33 |
| (1,83) | 1:71:A:LYS:C | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 10 | 1.33 |
| (1,60) | 1:60:A:LEU:N | 1:60:A:LEU:CA | 1:60:A:LEU:C | 1:61:A:LYS:N | 1 | 1.33 |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N | 1:170:A:SER:CA | 1:170:A:SER:C | 3 | 1.32 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 2 | 1.32 |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C | 1:138:A:GLU:N | 10 | 1.32 |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 9 | 1.32 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 10 | 1.32 |
| (1,97) | 1:78:A:GLN:C | 1:79:A:ILE:N | 1:79:A:ILE:CA | 1:79:A:ILE:C | 3 | 1.32 |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 1:136:A:PRO:N | 5 | 1.31 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 10 | 1.31 |
| (1,256) | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 1:168:A:PHE:N | 4 | 1.3 |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 9 | 1.3 |
| (1,133) | 1:99:A:LYS:C | 1:100:A:ALA:N | 1:100:A:ALA:CA | 1:100:A:ALA:C | 3 | 1.3 |
| (1,25) | 1:33:A:THR:C | 1:34:A:PRO:N | 1:34:A:PRO:CA | 1:34:A:PRO:C | 3 | 1.3 |
| (1,82) | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 1:72:A:PRO:N | 9 | 1.29 |
| (1,104) | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 1:83:A:SER:N | 7 | 1.28 |
| (1,75) | 1:67:A:ALA:C | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C | 1 | 1.28 |
| (1,49) | 1:54:A:GLN:C | 1:55:A:VAL:N | 1:55:A:VAL:CA | 1:55:A:VAL:C | 5 | 1.28 |
| (1,11) | 1:26:A:GLU:C | 1:27:A:SER:N | 1:27:A:SER:CA | 1:27:A:SER:C | 1 | 1.28 |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 9 | 1.27 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 10 | 1.27 |
| (1,189) | 1:130:A:ASN:C | 1:131:A:THR:N | 1:131:A:THR:CA | 1:131:A:THR:C | 1 | 1.27 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 6 | 1.27 |
| (1,52) | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C | 1:57:A:ASP:N | 7 | 1.27 |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C | 1:183:A:GLY:N | 3 | 1.26 |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N | 1:142:A:ILE:CA | 1:142:A:ILE:C | 4 | 1.26 |
| (1,58) | 1:59:A:LYS:N | 1:59:A:LYS:CA | 1:59:A:LYS:C | 1:60:A:LEU:N | 3 | 1.26 |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1 | 1.25 |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C | 1:138:A:GLU:N | 3 | 1.25 |
| (1,201) | 1:136:A:PRO:C | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C | 7 | 1.25 |
| (1,22) | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1:33:A:THR:N | 4 | 1.25 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 8 | 1.24 |
| (1,106) | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 1:84:A:GLY:N | 5 | 1.24 |
| (1,85) | 1:72:A:PRO:C | 1:73:A:TYR:N | 1:73:A:TYR:CA | 1:73:A:TYR:C | 6 | 1.24 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 5 | 1.23 |
| (1,36) | 1:46:A:TYR:N | 1:46:A:TYR:CA | 1:46:A:TYR:C | 1:47:A:ALA:N | 8 | 1.23 |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N | 1:174:A:ILE:CA | 1:174:A:ILE:C | 9 | 1.22 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1:167:A:LEU:N | 10 | 1.22 |
| (1,169) | 1:118:A:ILE:C | 1:119:A:ALA:N | 1:119:A:ALA:CA | 1:119:A:ALA:C | 9 | 1.22 |
| (1,106) | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 1:84:A:GLY:N | 8 | 1.22 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 6 | 1.22 |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1 | 1.21 |
| (1,215) | 1:146:A:ASN:C | 1:147:A:GLU:N | 1:147:A:GLU:CA | 1:147:A:GLU:C | 9 | 1.21 |
| (1,149) | 1:108:A:SER:C | 1:109:A:ALA:N | 1:109:A:ALA:CA | 1:109:A:ALA:C | 6 | 1.21 |
| (1,133) | 1:99:A:LYS:C | 1:100:A:ALA:N | 1:100:A:ALA:CA | 1:100:A:ALA:C | 4 | 1.21 |
| (1,131) | 1:98:A:THR:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 10 | 1.21 |
| (1,104) | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 1:83:A:SER:N | 4 | 1.21 |
| (1,84) | 1:72:A:PRO:N | 1:72:A:PRO:CA | 1:72:A:PRO:C | 1:73:A:TYR:N | 9 | 1.21 |
| (1,36) | 1:46:A:TYR:N | 1:46:A:TYR:CA | 1:46:A:TYR:C | 1:47:A:ALA:N | 2 | 1.21 |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N | 1:171:A:LEU:CA | 1:171:A:LEU:C | 7 | 1.2 |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1:167:A:LEU:N | 3 | 1.2 |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C | 1:130:A:ASN:N | 10 | 1.2 |
| (1,49) | 1:54:A:GLN:C | 1:55:A:VAL:N | 1:55:A:VAL:CA | 1:55:A:VAL:C | 6 | 1.2 |
| (1,46) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:LYS:N | 1 | 1.2 |
| (1,46) | 1:51:A:ILE:N | 1:51:A:ILE:CA | 1:51:A:ILE:C | 1:52:A:LYS:N | 3 | 1.2 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 2 | 1.2 |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C | 1:127:A:GLY:N | 6 | 1.19 |
| (1,159) | 1:113:A:LEU:C | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 4 | 1.19 |
| (1,137) | 1:101:A:VAL:C | 1:102:A:ILE:N | 1:102:A:ILE:CA | 1:102:A:ILE:C | 8 | 1.19 |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N | 1:145:A:TYR:CA | 1:145:A:TYR:C | 3 | 1.18 |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C | 1:138:A:GLU:N | 4 | 1.18 |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C | 7 | 1.18 |
| (1,118) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:ALA:N | 1 | 1.18 |
| (1,42) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:TRP:N | 2 | 1.18 |
| (1,36) | 1:46:A:TYR:N | 1:46:A:TYR:CA | 1:46:A:TYR:C | 1:47:A:ALA:N | 9 | 1.18 |
| (1,195) | 1:133:A:ILE:C | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 7 | 1.17 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 6 | 1.17 |
| (1,73) | 1:66:A:ASN:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 10 | 1.17 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 10 | 1.17 |
| (1,22) | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1:33:A:THR:N | 3 | 1.17 |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C | 1:183:A:GLY:N | 5 | 1.16 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 7 | 1.16 |
| (1,140) | 1:103:A:SER:N | 1:103:A:SER:CA | 1:103:A:SER:C | 1:104:A:LEU:N | 4 | 1.16 |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C | 1:183:A:GLY:N | 4 | 1.15 |
| (1,173) | 1:120:A:VAL:C | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C | 6 | 1.15 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 10 | 1.15 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 6 | 1.15 |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 1:121:A:LEU:N | 2 | 1.14 |
| (1,275) | 1:177:A:PHE:C | 1:178:A:GLN:N | 1:178:A:GLN:CA | 1:178:A:GLN:C | 5 | 1.13 |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N | 1:174:A:ILE:CA | 1:174:A:ILE:C | 2 | 1.13 |
| (1,168) | 1:118:A:ILE:N | 1:118:A:ILE:CA | 1:118:A:ILE:C | 1:119:A:ALA:N | 6 | 1.13 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 1 | 1.13 |
| (1,119) | 1:90:A:THR:C | 1:91:A:ALA:N | 1:91:A:ALA:CA | 1:91:A:ALA:C | 1 | 1.13 |
| (1,3) | 1:22:A:PRO:C | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C | 1 | 1.12 |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C | 1:160:A:TYR:N | 4 | 1.11 |
| (1,49) | 1:54:A:GLN:C | 1:55:A:VAL:N | 1:55:A:VAL:CA | 1:55:A:VAL:C | 2 | 1.11 |
| (1,177) | 1:122:A:TYR:C | 1:123:A:PRO:N | 1:123:A:PRO:CA | 1:123:A:PRO:C | 3 | 1.1 |
| (1,148) | 1:108:A:SER:N | 1:108:A:SER:CA | 1:108:A:SER:C | 1:109:A:ALA:N | 7 | 1.1 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,81) | 1:70:A:LEU:C | 1:71:A:LYS:N | 1:71:A:LYS:CA | 1:71:A:LYS:C | 10 | 1.1 |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C | 1:183:A:GLY:N | 10 | 1.09 |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C | 1:127:A:GLY:N | 9 | 1.09 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 2 | 1.09 |
| (1,8) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C | 1:26:A:GLU:N | 8 | 1.09 |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C | 1:167:A:LEU:N | 2 | 1.08 |
| (1,212) | 1:144:A:VAL:N | 1:144:A:VAL:CA | 1:144:A:VAL:C | 1:145:A:TYR:N | 9 | 1.08 |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 7 | 1.08 |
| (1,122) | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 1:93:A:GLY:N | 3 | 1.08 |
| (1,92) | 1:76:A:TYR:N | 1:76:A:TYR:CA | 1:76:A:TYR:C | 1:77:A:LEU:N | 7 | 1.08 |
| (1,91) | 1:75:A:LYS:C | 1:76:A:TYR:N | 1:76:A:TYR:CA | 1:76:A:TYR:C | 2 | 1.08 |
| (1,61) | 1:60:A:LEU:C | 1:61:A:LYS:N | 1:61:A:LYS:CA | 1:61:A:LYS:C | 5 | 1.08 |
| (1,53) | 1:56:A:ASN:C | 1:57:A:ASP:N | 1:57:A:ASP:CA | 1:57:A:ASP:C | 6 | 1.08 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 3 | 1.07 |
| (1,98) | 1:79:A:ILE:N | 1:79:A:ILE:CA | 1:79:A:ILE:C | 1:80:A:GLN:N | 10 | 1.07 |
| (1,79) | 1:69:A:GLN:C | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 4 | 1.07 |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 6 | 1.06 |
| (1,73) | 1:66:A:ASN:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 8 | 1.06 |
| (1,42) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:TRP:N | 1 | 1.06 |
| (1,195) | 1:133:A:ILE:C | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C | 6 | 1.05 |
| (1,121) | 1:91:A:ALA:C | 1:92:A:LEU:N | 1:92:A:LEU:CA | 1:92:A:LEU:C | 10 | 1.05 |
| (1,69) | 1:64:A:LEU:C | 1:65:A:ALA:N | 1:65:A:ALA:CA | 1:65:A:ALA:C | 9 | 1.05 |
| (1,65) | 1:62:A:VAL:C | 1:63:A:THR:N | 1:63:A:THR:CA | 1:63:A:THR:C | 6 | 1.05 |
| (1,22) | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1:33:A:THR:N | 8 | 1.05 |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C | 1:162:A:ALA:N | 8 | 1.04 |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C | 3 | 1.04 |
| (1,179) | 1:123:A:PRO:C | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C | 2 | 1.04 |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C | 5 | 1.04 |
| (1,68) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1:65:A:ALA:N | 4 | 1.04 |
| (1,36) | 1:46:A:TYR:N | 1:46:A:TYR:CA | 1:46:A:TYR:C | 1:47:A:ALA:N | 3 | 1.04 |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C | 1:183:A:GLY:N | 7 | 1.03 |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C | 1:136:A:PRO:N | 10 | 1.03 |
| (1,117) | 1:89:A:SER:C | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 3 | 1.03 |
| (1,103) | 1:81:A:ILE:C | 1:82:A:THR:N | 1:82:A:THR:CA | 1:82:A:THR:C | 2 | 1.03 |
| (1,71) | 1:65:A:ALA:C | 1:66:A:ASN:N | 1:66:A:ASN:CA | 1:66:A:ASN:C | 2 | 1.03 |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 1:121:A:LEU:N | 10 | 1.02 |
| (1,169) | 1:118:A:ILE:C | 1:119:A:ALA:N | 1:119:A:ALA:CA | 1:119:A:ALA:C | 4 | 1.02 |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C | 9 | 1.02 |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C | 1:115:A:LYS:N | 3 | 1.02 |
| (1,146) | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C | 1:107:A:PRO:N | 7 | 1.02 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 8 | 1.02 |
| (1,87) | 1:73:A:TYR:C | 1:74:A:PHE:N | 1:74:A:PHE:CA | 1:74:A:PHE:C | 7 | 1.02 |
| (1,79) | 1:69:A:GLN:C | 1:70:A:LEU:N | 1:70:A:LEU:CA | 1:70:A:LEU:C | 8 | 1.02 |
| (1,257) | 1:167:A:LEU:C | 1:168:A:PHE:N | 1:168:A:PHE:CA | 1:168:A:PHE:C | 3 | 1.01 |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C | 1:127:A:GLY:N | 3 | 1.01 |
| (1,110) | 1:85:A:TYR:N | 1:85:A:TYR:CA | 1:85:A:TYR:C | 1:86:A:GLU:N | 2 | 1.01 |
| (1,105) | 1:82:A:THR:C | 1:83:A:SER:N | 1:83:A:SER:CA | 1:83:A:SER:C | 1 | 1.01 |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C | 1:183:A:GLY:N | 2 | 1.0 |
| (1,119) | 1:90:A:THR:C | 1:91:A:ALA:N | 1:91:A:ALA:CA | 1:91:A:ALA:C | 9 | 1.0 |
| (1,114) | 1:87:A:THR:N | 1:87:A:THR:CA | 1:87:A:THR:C | 1:88:A:ASN:N | 5 | 1.0 |