# Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 08:22 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 2KA1 |
| BMRB ID | : | 16012 |
| Title | : | Solution NMR structure of BNIP3 transmembrane peptide dimer in detergent micelles |
| Authors | : | Sulistijo, E.S.; MacKenzie, K.R. |
| Deposited on | : | 2008-10-30 |

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 (i) 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 (1)) were used in the production of this report:

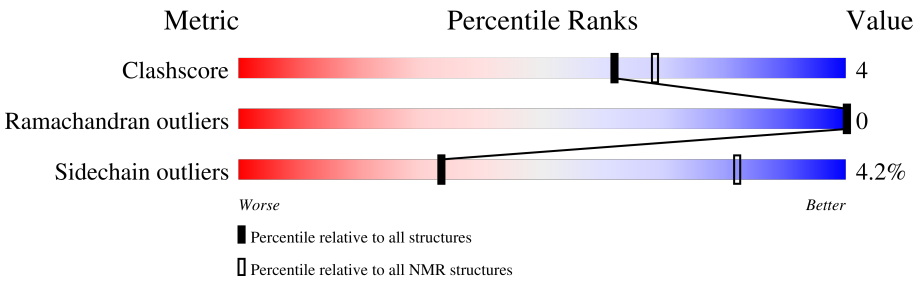
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.33 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 53%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 35 | 49% 9% 43% |
| 1 | B | 35 | 49% . 49% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 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:168-A:187, B:168-B:185 (38) | 0.46 | 8 |

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 8 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1132 atoms, of which 594 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BCL2/adenovirus E1B 19 kDa protein-interacting protein 3.

| Mol | Chain | Residues | Atoms | | | | | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | |
| 1 | A | 35 | 566 | 182 | 297 | 44 | 43 | 0 |
| 1 | B | 35 | 566 | 182 | 297 | 44 | 43 | 0 |

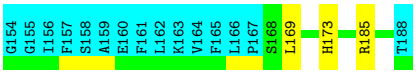
# 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

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

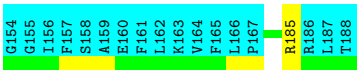
• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 49% 9% 43%




• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 49% • 49%




## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

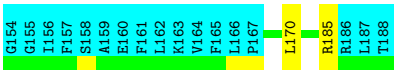
### 4.2.1 Score per residue for model 1

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 46% 11% 43%

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

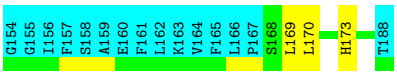
Chain B: 46% 6% 49%



### 4.2.2 Score per residue for model 2

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 49% 9% 43%



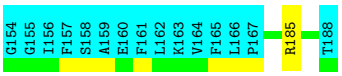

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 37% 14% 49%

### 4.2.3 Score per residue for model 3

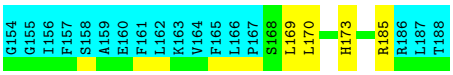
• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 54% • 43%




• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

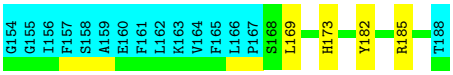
Chain B: 40% 11% 49%




### 4.2.4 Score per residue for model 4

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 46% 11% 43%




• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 43% 9% 49%

### 4.2.5 Score per residue for model 5

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 43% 14% 43%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 S168 L169 L170 H173 G180 R185 T188

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 46% 6% 49%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 L170 I181 R186 L187 T188

### 4.2.6 Score per residue for model 6

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 43% 14% 43%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 L179 G180 I181 Y182 I183 G184 R185 T188

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 37% 14% 49%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 S168 L169 L170 H173 G180 R185 R186 L187 T188

### 4.2.7 Score per residue for model 7

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 49% 9% 43%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 S168 L169 L170 H173 T188

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 51% 49%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 R186 L187 T188

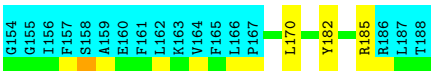
### 4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 46% 11% 43%

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

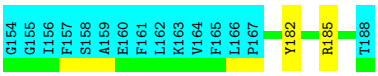
Chain B: 43% 9% 49%




### 4.2.9 Score per residue for model 9

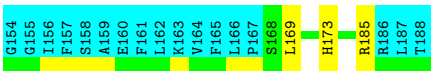
• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 51% 6% 43%




• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 43% 9% 49%



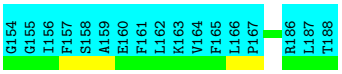

### 4.2.10 Score per residue for model 10

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 43% 14% 43%

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

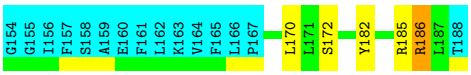
Chain B: 51% 49%



### 4.2.11 Score per residue for model 11

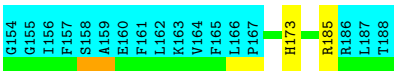
- Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 43% 11% • 43%




- Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

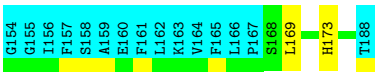
Chain B: 46% 6% 49%




### 4.2.12 Score per residue for model 12

- Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 51% 6% 43%




- Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 43% 9% 49%

### 4.2.13 Score per residue for model 13

- Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 46% 11% 43%

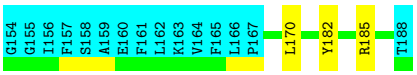
- Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 43% 9% 49%

### 4.2.14 Score per residue for model 14

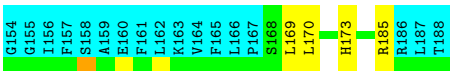
• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 49% 9% 43%




• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 40% 11% 49%



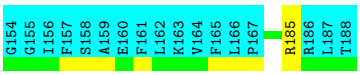

### 4.2.15 Score per residue for model 15

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 46% 11% 43%

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

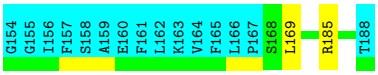
Chain B: 49% • 49%




### 4.2.16 Score per residue for model 16

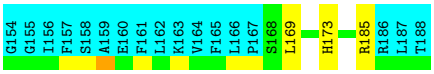
• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 51% 6% 43%




• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 43% 9% 49%



### 4.2.17 Score per residue for model 17

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 49% 9% 43%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 S168 L169 L170 R185 T188

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 49% • 49%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 R185 R186 L187 T188

### 4.2.18 Score per residue for model 18

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 51% 6% 43%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 S168 L169 H173 T188

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B: 46% 6% 49%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 L179 I183 R186 L187 T188

### 4.2.19 Score per residue for model 19

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A: 54% • 43%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 R186 L187 T188

• Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

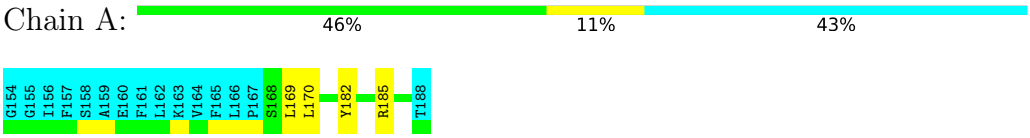
Chain B: 49% • 49%

G154 G155 I156 F157 S158 A159 E160 F161 L162 K163 V164 F165 L166 P167 R185 R186 L187 T188

### 4.2.20 Score per residue for model 20

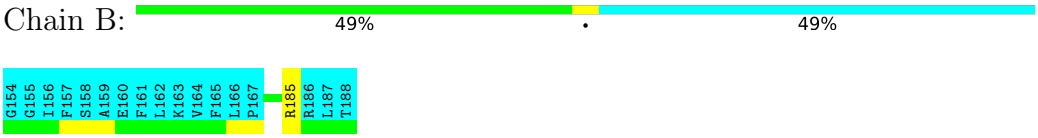
- Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain A:




- Molecule 1: BCL2/adenovirus E1B 19 kDa protein-interacting protein 3

Chain B:



# 5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *lowest energy*.

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

| Software name | Classification | Version |
|---|---|---|
| ARIA | refinement | 1.2 |
| ARIA | structure solution | 1.2 |

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 | 501 |
| Number of shifts mapped to atoms | 501 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 53% |

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 153 | 177 | 176 | 2±1 |
| 1 | B | 134 | 153 | 152 | 1±1 |
| All | All | 5740 | 6600 | 6560 | 55 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:181:ILE:HD13 | 1:B:180:GLY:O | 0.51 | 2.06 | 6 | 1 |
| 1:A:182:TYR:CE2 | 1:A:186:ARG:NH2 | 0.51 | 2.79 | 10 | 1 |
| 1:A:182:TYR:CZ | 1:A:186:ARG:CZ | 0.50 | 2.93 | 10 | 1 |
| 1:A:182:TYR:CE2 | 1:A:186:ARG:CZ | 0.46 | 2.99 | 10 | 1 |
| 1:A:181:ILE:HD12 | 1:A:181:ILE:N | 0.46 | 2.26 | 13 | 1 |
| 1:A:170:LEU:CD1 | 1:A:170:LEU:N | 0.44 | 2.80 | 20 | 2 |
| 1:A:170:LEU:N | 1:A:170:LEU:HD12 | 0.43 | 2.29 | 11 | 8 |
| 1:B:170:LEU:N | 1:B:170:LEU:HD12 | 0.43 | 2.29 | 8 | 6 |
| 1:B:182:TYR:O | 1:B:185:ARG:CG | 0.43 | 2.67 | 2 | 1 |
| 1:A:172:SER:HB3 | 1:B:173:HIS:CD2 | 0.43 | 2.49 | 13 | 2 |
| 1:B:170:LEU:N | 1:B:170:LEU:CD1 | 0.43 | 2.82 | 13 | 1 |
| 1:A:169:LEU:O | 1:A:173:HIS:ND1 | 0.42 | 2.52 | 15 | 11 |
| 1:B:169:LEU:O | 1:B:173:HIS:ND1 | 0.42 | 2.53 | 6 | 8 |

*Continued on next page...*

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:182:TYR:O | 1:A:185:ARG:CG | 0.42 | 2.68 | 9 | 6 |
| 1:B:179:LEU:O | 1:B:183:ILE:CD1 | 0.42 | 2.67 | 18 | 1 |
| 1:A:182:TYR:CE2 | 1:A:186:ARG:NE | 0.41 | 2.88 | 11 | 1 |
| 1:B:179:LEU:O | 1:B:183:ILE:HD12 | 0.41 | 2.15 | 18 | 1 |
| 1:A:180:GLY:CA | 1:B:181:ILE:HG13 | 0.41 | 2.46 | 5 | 1 |
| 1:A:179:LEU:O | 1:A:183:ILE:CD1 | 0.40 | 2.70 | 6 | 1 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 20/35 (57%) | 19±1 (96±3%) | 1±1 (4±3%) | 0±0 (0±0%) | 100 | 100 |
| 1 | B | 18/35 (51%) | 18±0 (100±0%) | 0±0 (0±0%) | 0±0 (0±0%) | 100 | 100 |
| All | All | 760/1400 (54%) | 742 (98%) | 18 (2%) | 0 (0%) | 100 | 100 |

There are no Ramachandran outliers.

### 6.3.2 Protein sidechains (i)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 16/28 (57%) | 15±1 (97±4%) | 1±1 (3±4%) | 40 | 87 |
| 1 | B | 14/28 (50%) | 13±0 (95±3%) | 1±0 (5±3%) | 28 | 77 |
| All | All | 600/1120 (54%) | 575 (96%) | 25 (4%) | 33 | 82 |

All 4 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 | B | 185 | ARG | 14 |
| 1 | A | 185 | ARG | 8 |
| 1 | A | 186 | ARG | 2 |
| 1 | A | 170 | LEU | 1 |

#### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry (i)

There are no ligands in this entry.

### 6.7 Other polymers (i)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 49% for the entire structure.

## 7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

### 7.1.1 Bookkeeping (i)

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

| | |
|---|---|
| Total number of shifts | 501 |
| Number of shifts mapped to atoms | 501 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 35 | -0.46 ± 0.29 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 30 | 0.68 ± 0.09 | Should be checked |
| $^{13}C'$ | 33 | 0.70 ± 0.31 | Should be applied |
| $^{15}N$ | 33 | 0.96 ± 0.28 | Should be applied |

### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 53%, i.e. 297 atoms were assigned a chemical shift out of a possible 563. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 103/196 (53%) | 43/82 (52%) | 40/76 (53%) | 20/38 (53%) |
| Sidechain | 182/333 (55%) | 123/226 (54%) | 53/98 (54%) | 6/9 (67%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 12/34 (35%) | 6/16 (38%) | 6/14 (43%) | 0/4 (0%) |
| Overall | 297/563 (53%) | 172/324 (53%) | 99/188 (53%) | 26/51 (51%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 496 atoms were assigned a chemical shift out of a possible 1014. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 174/356 (49%) | 73/148 (49%) | 68/140 (49%) | 33/68 (49%) |
| Sidechain | 280/564 (50%) | 190/380 (50%) | 84/170 (49%) | 6/14 (43%) |
| Aromatic | 42/94 (45%) | 21/46 (46%) | 21/44 (48%) | 0/4 (0%) |
| Overall | 496/1014 (49%) | 284/574 (49%) | 173/354 (49%) | 39/86 (45%) |

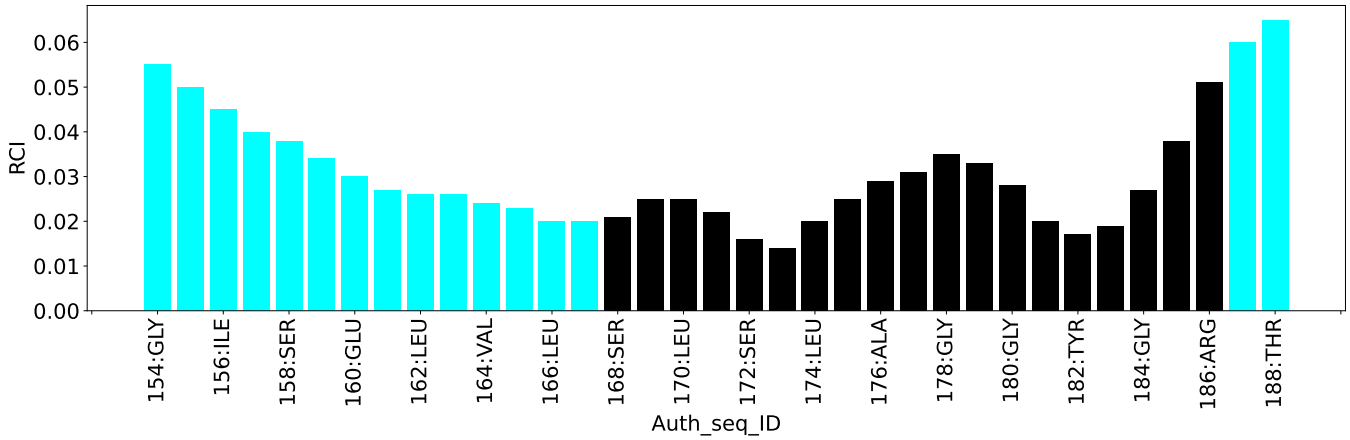
### 7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



# 8 NMR restraints analysis (i)

## 8.1 Conformationally restricting restraints (i)

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 | 2032 |
| Intra-residue (\|i-j\|=0) | 1251 |
| Sequential (\|i-j\|=1) | 401 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 376 |
| Long range (\|i-j\|≥5) | 4 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 29.0 |
| Number of long range restraints per residue[1] | 0.1 |

[1]Long 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 (i)

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 (i)

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) | 17.6 | 0.2 |
| 0.2-0.5 (Medium) | 19.1 | 0.5 |
| >0.5 (Large) | 50.7 | 4.26 |

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

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

# 9 Distance violation analysis (i)

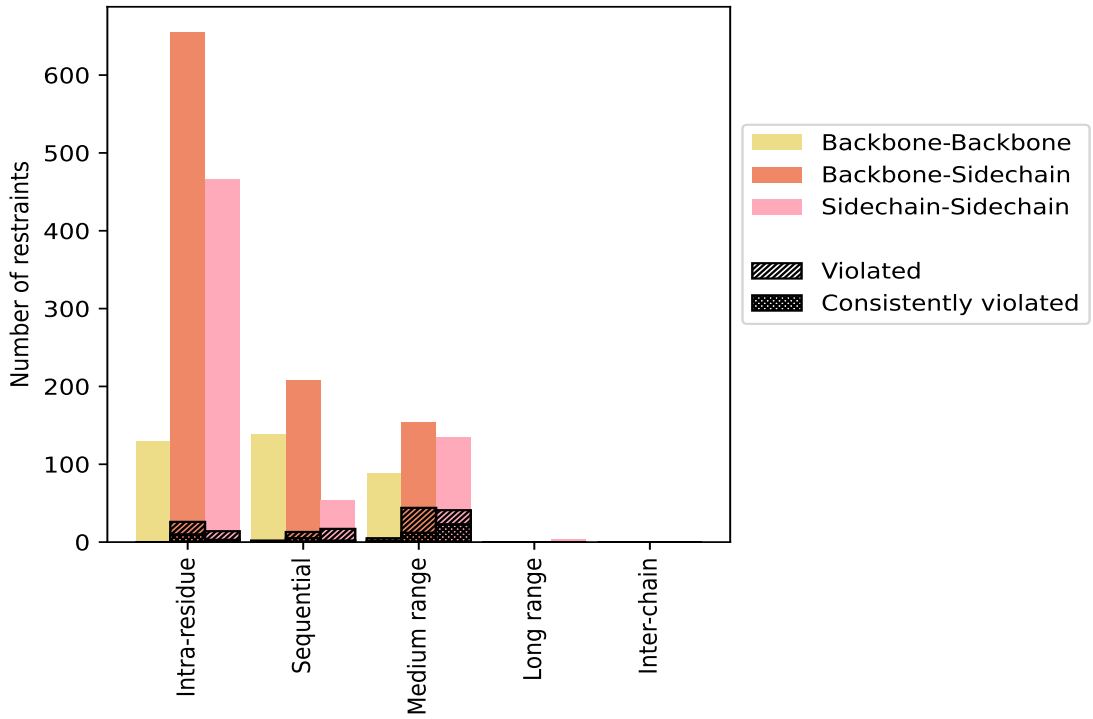
## 9.1 Summary of distance violations (i)

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

| Restraints type | Count | %[1] | Violated[3] | | | Consistently Violated[4] | | |
|---|---|---|---|---|---|---|---|---|
| | | | Count | %[2] | %[1] | Count | %[2] | %[1] |
| Intra-residue (\|i-j\|=0) | 1251 | 61.6 | 40 | 3.2 | 2.0 | 13 | 1.0 | 0.6 |
| Backbone-Backbone | 130 | 6.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 655 | 32.2 | 26 | 4.0 | 1.3 | 10 | 1.5 | 0.5 |
| Sidechain-Sidechain | 466 | 22.9 | 14 | 3.0 | 0.7 | 3 | 0.6 | 0.1 |
| Sequential (\|i-j\|=1) | 401 | 19.7 | 32 | 8.0 | 1.6 | 7 | 1.7 | 0.3 |
| Backbone-Backbone | 139 | 6.8 | 2 | 1.4 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 208 | 10.2 | 13 | 6.2 | 0.6 | 5 | 2.4 | 0.2 |
| Sidechain-Sidechain | 54 | 2.7 | 17 | 31.5 | 0.8 | 2 | 3.7 | 0.1 |
| Medium range (\|i-j\|>1 & \|i-j\|<5) | 376 | 18.5 | 90 | 23.9 | 4.4 | 37 | 9.8 | 1.8 |
| Backbone-Backbone | 88 | 4.3 | 5 | 5.7 | 0.2 | 2 | 2.3 | 0.1 |
| Backbone-Sidechain | 154 | 7.6 | 44 | 28.6 | 2.2 | 12 | 7.8 | 0.6 |
| Sidechain-Sidechain | 134 | 6.6 | 41 | 30.6 | 2.0 | 23 | 17.2 | 1.1 |
| Long range (\|i-j\|≥5) | 4 | 0.2 | 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 | 4 | 0.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 2032 | 100.0 | 162 | 8.0 | 8.0 | 57 | 2.8 | 2.8 |
| Backbone-Backbone | 357 | 17.6 | 7 | 2.0 | 0.3 | 2 | 0.6 | 0.1 |
| Backbone-Sidechain | 1017 | 50.0 | 83 | 8.2 | 4.1 | 27 | 2.7 | 1.3 |
| Sidechain-Sidechain | 658 | 32.4 | 72 | 10.9 | 3.5 | 28 | 4.3 | 1.4 |

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

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




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

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

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 1 | 18 | 14 | 54 | 0 | 0 | 86 | 0.95 | 4.13 | 1.03 | 0.69 |
| 2 | 20 | 18 | 56 | 0 | 0 | 94 | 1.0 | 4.08 | 1.02 | 0.66 |
| 3 | 19 | 12 | 54 | 0 | 0 | 85 | 1.0 | 4.1 | 1.02 | 0.69 |
| 4 | 17 | 12 | 53 | 0 | 0 | 82 | 0.98 | 4.02 | 1.01 | 0.6 |
| 5 | 18 | 14 | 50 | 0 | 0 | 82 | 0.94 | 4.04 | 1.04 | 0.52 |
| 6 | 19 | 15 | 56 | 0 | 0 | 90 | 0.94 | 4.04 | 1.02 | 0.62 |
| 7 | 21 | 20 | 50 | 0 | 0 | 91 | 0.97 | 4.05 | 1.0 | 0.64 |
| 8 | 19 | 14 | 52 | 0 | 0 | 85 | 1.06 | 4.04 | 1.06 | 0.71 |
| 9 | 19 | 9 | 51 | 0 | 0 | 79 | 1.05 | 4.26 | 1.13 | 0.66 |
| 10 | 17 | 19 | 58 | 0 | 0 | 94 | 0.97 | 3.94 | 0.96 | 0.64 |
| 11 | 20 | 16 | 57 | 0 | 0 | 93 | 0.93 | 4.18 | 1.04 | 0.64 |

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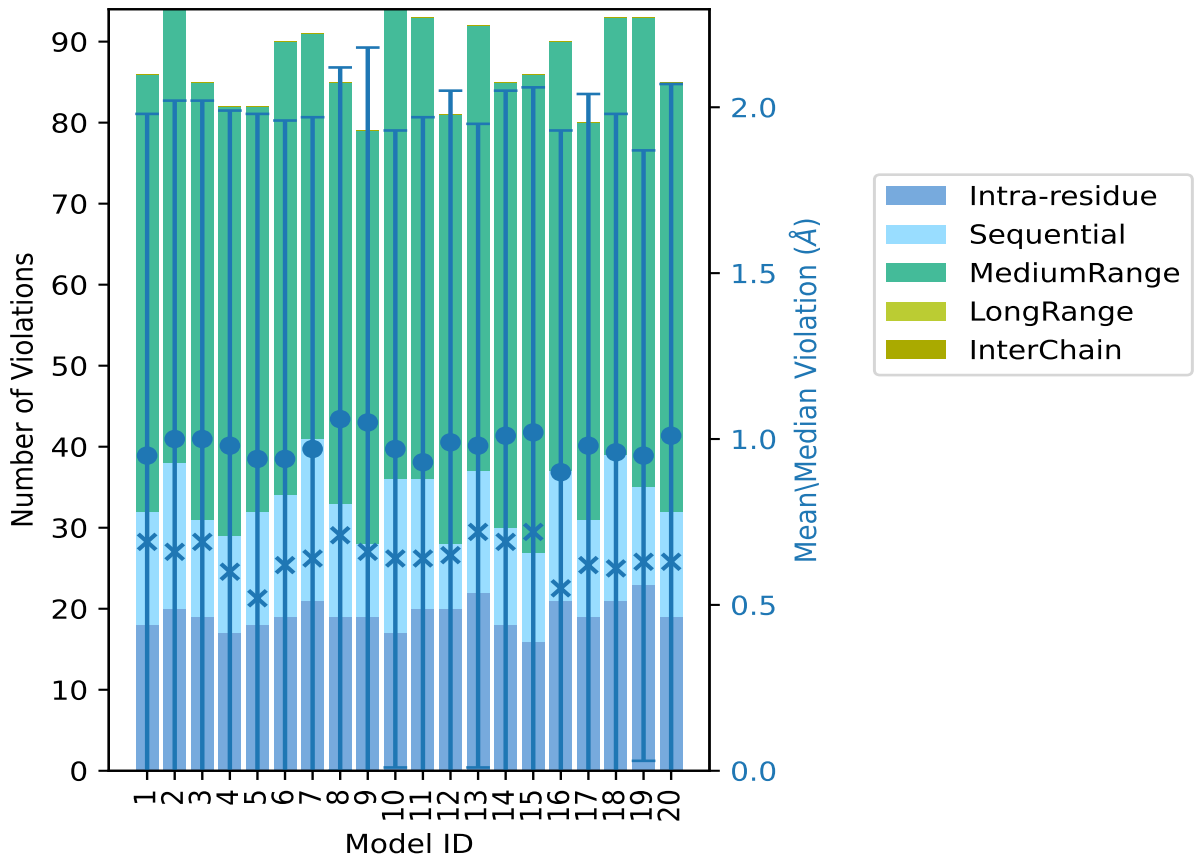
| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 12 | 20 | 8 | 53 | 0 | 0 | 81 | 0.99 | 4.13 | 1.06 | 0.65 |
| 13 | 22 | 15 | 55 | 0 | 0 | 92 | 0.98 | 3.97 | 0.97 | 0.72 |
| 14 | 18 | 12 | 55 | 0 | 0 | 85 | 1.01 | 4.03 | 1.04 | 0.69 |
| 15 | 16 | 11 | 59 | 0 | 0 | 86 | 1.02 | 4.04 | 1.04 | 0.72 |
| 16 | 21 | 16 | 53 | 0 | 0 | 90 | 0.9 | 4.16 | 1.03 | 0.55 |
| 17 | 19 | 12 | 49 | 0 | 0 | 80 | 0.98 | 4.12 | 1.06 | 0.62 |
| 18 | 21 | 18 | 54 | 0 | 0 | 93 | 0.96 | 4.03 | 1.02 | 0.61 |
| 19 | 23 | 12 | 58 | 0 | 0 | 93 | 0.95 | 3.98 | 0.92 | 0.63 |
| 20 | 19 | 13 | 53 | 0 | 0 | 85 | 1.01 | 4.11 | 1.06 | 0.63 |

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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

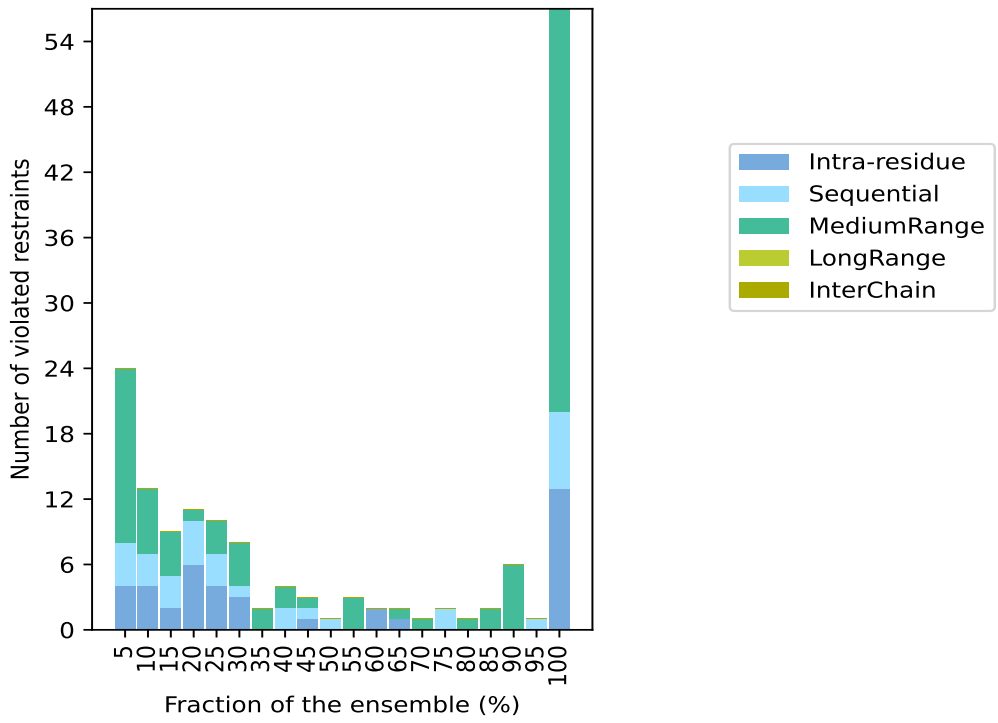
## 9.3 Distance violation statistics for the ensemble (i)

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, 1870(IR:1211, SQ:369, MR:286, LR:4, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|---|---|---|---|---|---|---|---|
| IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | Count[6] | % |
| 4 | 4 | 16 | 0 | 0 | 24 | 1 | 5.0 |
| 4 | 3 | 6 | 0 | 0 | 13 | 2 | 10.0 |
| 2 | 3 | 4 | 0 | 0 | 9 | 3 | 15.0 |
| 6 | 4 | 1 | 0 | 0 | 11 | 4 | 20.0 |
| 4 | 3 | 3 | 0 | 0 | 10 | 5 | 25.0 |
| 3 | 1 | 4 | 0 | 0 | 8 | 6 | 30.0 |
| 0 | 0 | 2 | 0 | 0 | 2 | 7 | 35.0 |
| 0 | 2 | 2 | 0 | 0 | 4 | 8 | 40.0 |
| 1 | 1 | 1 | 0 | 0 | 3 | 9 | 45.0 |
| 0 | 1 | 0 | 0 | 0 | 1 | 10 | 50.0 |
| 0 | 0 | 3 | 0 | 0 | 3 | 11 | 55.0 |
| 2 | 0 | 0 | 0 | 0 | 2 | 12 | 60.0 |
| 1 | 0 | 1 | 0 | 0 | 2 | 13 | 65.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 14 | 70.0 |
| 0 | 2 | 0 | 0 | 0 | 2 | 15 | 75.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 16 | 80.0 |
| 0 | 0 | 2 | 0 | 0 | 2 | 17 | 85.0 |
| 0 | 0 | 6 | 0 | 0 | 6 | 18 | 90.0 |
| 0 | 1 | 0 | 0 | 0 | 1 | 19 | 95.0 |
| 13 | 7 | 37 | 0 | 0 | 57 | 20 | 100.0 |

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

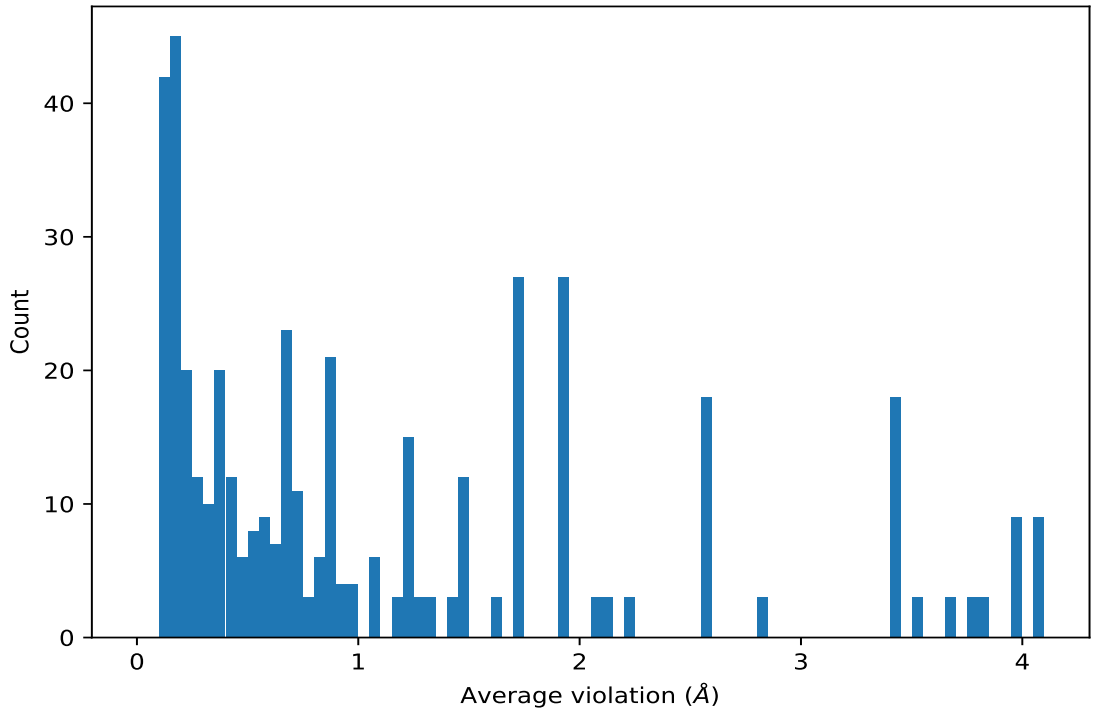
### 9.3.1 Bar graph : Distance violation statistics for the ensemble (i)




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

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

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




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

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

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 20 | 4.05 | 0.11 | 4.04 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 20 | 3.95 | 0.11 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 20 | 3.95 | 0.11 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 20 | 3.95 | 0.11 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 20 | 3.95 | 0.11 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 20 | 3.95 | 0.11 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 20 | 3.95 | 0.11 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 20 | 3.95 | 0.11 | 3.94 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 20 | 3.95 | 0.11 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 20 | 3.95 | 0.11 | 3.94 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 20 | 3.84 | 0.4 | 3.97 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 20 | 3.84 | 0.4 | 3.97 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 20 | 3.84 | 0.4 | 3.97 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 20 | 3.76 | 0.15 | 3.78 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 20 | 3.76 | 0.15 | 3.78 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 20 | 3.76 | 0.15 | 3.78 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 20 | 3.66 | 0.15 | 3.68 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 20 | 3.66 | 0.15 | 3.68 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 20 | 3.66 | 0.15 | 3.68 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 20 | 3.54 | 0.4 | 3.67 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 20 | 3.54 | 0.4 | 3.67 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 20 | 3.54 | 0.4 | 3.67 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 20 | 3.43 | 0.09 | 3.46 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 20 | 2.84 | 0.4 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 20 | 2.84 | 0.4 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 20 | 2.84 | 0.4 | 2.97 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 20 | 2.57 | 0.09 | 2.58 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 20 | 2.57 | 0.09 | 2.58 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 20 | 2.24 | 0.4 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 20 | 2.24 | 0.4 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 20 | 2.24 | 0.4 | 2.37 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 20 | 2.13 | 0.1 | 2.11 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 20 | 2.13 | 0.1 | 2.11 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 20 | 2.13 | 0.1 | 2.11 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 20 | 2.06 | 0.49 | 2.22 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 20 | 2.06 | 0.49 | 2.22 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 20 | 2.06 | 0.49 | 2.22 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 20 | 1.9 | 0.16 | 1.92 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 20 | 1.9 | 0.16 | 1.92 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 20 | 1.7 | 0.16 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 20 | 1.7 | 0.16 | 1.72 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 20 | 1.63 | 0.1 | 1.61 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 20 | 1.63 | 0.1 | 1.61 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 20 | 1.63 | 0.1 | 1.61 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 20 | 1.49 | 0.12 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 20 | 1.49 | 0.12 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 20 | 1.49 | 0.12 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 20 | 1.49 | 0.12 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 20 | 1.49 | 0.12 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 20 | 1.49 | 0.12 | 1.52 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 20 | 1.3 | 0.54 | 1.39 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 20 | 1.28 | 0.14 | 1.26 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 20 | 1.28 | 0.14 | 1.26 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 20 | 1.28 | 0.14 | 1.26 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 20 | 1.22 | 1.04 | 0.69 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 20 | 1.22 | 1.04 | 0.69 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 20 | 1.22 | 1.04 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 20 | 1.22 | 1.04 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 20 | 1.22 | 1.04 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 20 | 1.22 | 1.04 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 20 | 1.22 | 1.04 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 20 | 1.22 | 1.04 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 20 | 1.22 | 1.04 | 0.69 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 20 | 1.21 | 0.34 | 1.19 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 20 | 1.18 | 0.14 | 1.16 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 20 | 1.18 | 0.14 | 1.16 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 20 | 1.18 | 0.14 | 1.16 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 20 | 1.07 | 0.02 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 20 | 1.07 | 0.02 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 20 | 1.07 | 0.02 | 1.07 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 20 | 0.99 | 0.52 | 0.82 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 20 | 0.89 | 0.19 | 0.86 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 20 | 0.89 | 0.19 | 0.86 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 20 | 0.89 | 0.19 | 0.86 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 20 | 0.89 | 0.19 | 0.86 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 20 | 0.89 | 0.19 | 0.86 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 20 | 0.89 | 0.19 | 0.86 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 20 | 0.89 | 0.12 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 20 | 0.89 | 0.12 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 20 | 0.89 | 0.12 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 20 | 0.89 | 0.12 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 20 | 0.89 | 0.12 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 20 | 0.89 | 0.12 | 0.92 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 20 | 0.87 | 0.02 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 20 | 0.87 | 0.02 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 20 | 0.87 | 0.02 | 0.87 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 20 | 0.87 | 0.08 | 0.88 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 20 | 0.87 | 0.08 | 0.88 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 20 | 0.87 | 0.08 | 0.88 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 20 | 0.87 | 0.08 | 0.88 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 20 | 0.87 | 0.08 | 0.88 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 20 | 0.87 | 0.08 | 0.88 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 20 | 0.84 | 0.11 | 0.86 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 20 | 0.84 | 0.11 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 20 | 0.84 | 0.11 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 20 | 0.84 | 0.11 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 20 | 0.84 | 0.11 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 20 | 0.84 | 0.11 | 0.86 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 20 | 0.79 | 0.0 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 20 | 0.79 | 0.0 | 0.79 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 20 | 0.76 | 0.08 | 0.75 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 20 | 0.69 | 0.19 | 0.66 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 20 | 0.69 | 0.19 | 0.66 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 20 | 0.69 | 0.19 | 0.66 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 20 | 0.67 | 0.08 | 0.68 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 20 | 0.67 | 0.08 | 0.68 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 20 | 0.67 | 0.08 | 0.68 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 20 | 0.67 | 0.08 | 0.68 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 20 | 0.67 | 0.08 | 0.68 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 20 | 0.67 | 0.08 | 0.68 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 20 | 0.67 | 0.04 | 0.66 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 20 | 0.67 | 0.04 | 0.66 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 20 | 0.67 | 0.04 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 20 | 0.67 | 0.04 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 20 | 0.67 | 0.04 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 20 | 0.67 | 0.04 | 0.66 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 20 | 0.66 | 0.05 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 20 | 0.66 | 0.05 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 20 | 0.66 | 0.05 | 0.64 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 20 | 0.56 | 0.08 | 0.55 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 20 | 0.56 | 0.11 | 0.61 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 20 | 0.56 | 0.11 | 0.61 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 20 | 0.47 | 0.02 | 0.47 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 20 | 0.47 | 0.02 | 0.47 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 20 | 0.47 | 0.02 | 0.47 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 20 | 0.47 | 0.02 | 0.47 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 20 | 0.47 | 0.02 | 0.47 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 20 | 0.47 | 0.02 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 20 | 0.44 | 0.06 | 0.46 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 20 | 0.44 | 0.06 | 0.46 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 20 | 0.44 | 0.06 | 0.46 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 20 | 0.39 | 0.0 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 20 | 0.39 | 0.0 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 20 | 0.39 | 0.0 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 20 | 0.39 | 0.0 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 20 | 0.39 | 0.0 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 20 | 0.39 | 0.0 | 0.39 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 20 | 0.36 | 0.05 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 20 | 0.36 | 0.05 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 20 | 0.36 | 0.05 | 0.34 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 20 | 0.27 | 0.05 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 20 | 0.27 | 0.05 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 20 | 0.27 | 0.05 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 20 | 0.27 | 0.05 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 20 | 0.27 | 0.05 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 20 | 0.27 | 0.05 | 0.28 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 20 | 0.22 | 0.0 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 20 | 0.22 | 0.0 | 0.22 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 20 | 0.19 | 0.0 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 20 | 0.19 | 0.0 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 20 | 0.19 | 0.0 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 20 | 0.19 | 0.0 | 0.19 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 20 | 0.14 | 0.0 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 20 | 0.14 | 0.0 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 20 | 0.14 | 0.0 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 20 | 0.14 | 0.0 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 20 | 0.14 | 0.0 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 20 | 0.14 | 0.0 | 0.14 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 19 | 0.64 | 0.32 | 0.61 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 18 | 1.43 | 0.34 | 1.48 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 18 | 1.43 | 0.34 | 1.48 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 18 | 1.43 | 0.34 | 1.48 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 18 | 1.23 | 0.34 | 1.27 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 18 | 1.23 | 0.34 | 1.27 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 18 | 1.23 | 0.34 | 1.27 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 18 | 0.5 | 0.05 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 18 | 0.5 | 0.05 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 18 | 0.5 | 0.05 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 18 | 0.5 | 0.05 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 18 | 0.5 | 0.05 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 18 | 0.5 | 0.05 | 0.5 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 18 | 0.32 | 0.17 | 0.31 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 18 | 0.17 | 0.05 | 0.15 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 18 | 0.17 | 0.05 | 0.15 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 18 | 0.17 | 0.05 | 0.15 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 18 | 0.17 | 0.05 | 0.15 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 18 | 0.17 | 0.05 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 18 | 0.17 | 0.05 | 0.15 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 17 | 0.55 | 0.26 | 0.51 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 17 | 0.55 | 0.26 | 0.51 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 17 | 0.55 | 0.26 | 0.51 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 17 | 0.34 | 0.17 | 0.29 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 17 | 0.34 | 0.17 | 0.29 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 17 | 0.34 | 0.17 | 0.29 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 16 | 0.95 | 0.76 | 0.68 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 16 | 0.95 | 0.76 | 0.68 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 16 | 0.95 | 0.76 | 0.68 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 15 | 0.2 | 0.05 | 0.2 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 15 | 0.2 | 0.05 | 0.2 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 14 | 0.6 | 0.3 | 0.59 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 13 | 0.23 | 0.12 | 0.19 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 13 | 0.23 | 0.12 | 0.19 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 13 | 0.23 | 0.12 | 0.19 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 13 | 0.18 | 0.03 | 0.19 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 12 | 0.28 | 0.03 | 0.28 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 12 | 0.17 | 0.01 | 0.16 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 11 | 1.07 | 0.71 | 1.02 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 11 | 1.07 | 0.71 | 1.02 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 11 | 1.07 | 0.71 | 1.02 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 11 | 0.15 | 0.04 | 0.15 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 10 | 0.37 | 0.25 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 10 | 0.37 | 0.25 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 10 | 0.37 | 0.25 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 10 | 0.37 | 0.25 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 10 | 0.37 | 0.25 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 10 | 0.37 | 0.25 | 0.28 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 9 | 0.3 | 0.13 | 0.39 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 9 | 0.27 | 0.08 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 9 | 0.27 | 0.08 | 0.26 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 9 | 0.27 | 0.08 | 0.26 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 9 | 0.22 | 0.04 | 0.22 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 9 | 0.22 | 0.04 | 0.22 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 9 | 0.22 | 0.04 | 0.22 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 8 | 0.62 | 0.2 | 0.66 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 8 | 0.4 | 0.24 | 0.38 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 8 | 0.4 | 0.24 | 0.38 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 8 | 0.4 | 0.24 | 0.38 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 8 | 0.4 | 0.24 | 0.38 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 8 | 0.4 | 0.24 | 0.38 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 8 | 0.4 | 0.24 | 0.38 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 8 | 0.2 | 0.1 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 8 | 0.2 | 0.1 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 8 | 0.2 | 0.1 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 8 | 0.2 | 0.1 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 8 | 0.2 | 0.1 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 8 | 0.2 | 0.1 | 0.15 |
| (1,1691) | 1:B:158:SER:H | 1:B:162:LEU:HG | 7 | 0.58 | 0.25 | 0.65 |
| (1,1699) | 1:B:160:GLU:H | 1:B:158:SER:HB3 | 7 | 0.36 | 0.14 | 0.42 |
| (1,846) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 6 | 0.93 | 0.49 | 0.88 |
| (1,1425) | 1:B:158:SER:H | 1:B:162:LEU:HG | 6 | 0.56 | 0.19 | 0.62 |
| (1,572) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 6 | 0.51 | 0.0 | 0.51 |
| (1,1698) | 1:B:160:GLU:H | 1:B:158:SER:HB2 | 6 | 0.35 | 0.33 | 0.12 |
| (1,104) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 6 | 0.31 | 0.0 | 0.31 |
| (1,1579) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 6 | 0.19 | 0.05 | 0.18 |
| (1,1848) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 6 | 0.19 | 0.05 | 0.18 |
| (1,96) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HB2 | 6 | 0.13 | 0.01 | 0.12 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 5 | 1.47 | 0.4 | 1.54 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 5 | 1.47 | 0.4 | 1.54 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 5 | 1.47 | 0.4 | 1.54 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 5 | 1.47 | 0.4 | 1.54 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 5 | 1.47 | 0.4 | 1.54 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 5 | 1.47 | 0.4 | 1.54 |
| (1,377) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 5 | 0.74 | 0.46 | 0.95 |
| (1,1159) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 5 | 0.58 | 0.29 | 0.68 |
| (1,1670) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 5 | 0.36 | 0.0 | 0.36 |
| (2,26) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 5 | 0.35 | 0.26 | 0.25 |
| (2,30) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 5 | 0.35 | 0.26 | 0.25 |
| (1,148) | 1:B:166:LEU:HB3 | 1:B:167:PRO:HD2 | 5 | 0.23 | 0.04 | 0.22 |
| (1,1405) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 5 | 0.16 | 0.0 | 0.16 |
| (1,387) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 5 | 0.12 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,856) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 5 | 0.12 | 0.01 | 0.12 |
| (1,437) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 4 | 0.9 | 0.26 | 0.84 |
| (1,437) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 4 | 0.9 | 0.26 | 0.84 |
| (1,437) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 4 | 0.9 | 0.26 | 0.84 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 4 | 0.7 | 0.32 | 0.58 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 4 | 0.7 | 0.32 | 0.58 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 4 | 0.7 | 0.32 | 0.58 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 4 | 0.7 | 0.32 | 0.58 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 4 | 0.7 | 0.32 | 0.58 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 4 | 0.7 | 0.32 | 0.58 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 4 | 0.7 | 0.32 | 0.58 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 4 | 0.7 | 0.32 | 0.58 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 4 | 0.7 | 0.32 | 0.58 |
| (1,903) | 1:B:188:THR:HG21 | 1:B:187:LEU:H | 4 | 0.65 | 0.1 | 0.68 |
| (1,903) | 1:B:188:THR:HG22 | 1:B:187:LEU:H | 4 | 0.65 | 0.1 | 0.68 |
| (1,903) | 1:B:188:THR:HG23 | 1:B:187:LEU:H | 4 | 0.65 | 0.1 | 0.68 |
| (1,970) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 4 | 0.4 | 0.19 | 0.4 |
| (1,1888) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 4 | 0.31 | 0.01 | 0.3 |
| (1,1462) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 4 | 0.29 | 0.0 | 0.29 |
| (1,1730) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 4 | 0.29 | 0.0 | 0.29 |
| (1,105) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HB3 | 4 | 0.21 | 0.06 | 0.19 |
| (1,1619) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 4 | 0.21 | 0.01 | 0.2 |
| (1,1419) | 1:B:158:SER:H | 1:B:158:SER:HB2 | 4 | 0.18 | 0.01 | 0.18 |
| (1,1400) | 1:B:156:ILE:H | 1:B:155:GLY:HA3 | 4 | 0.13 | 0.02 | 0.12 |
| (1,1359) | 1:B:157:PHE:HD1 | 1:B:160:GLU:HB2 | 3 | 1.31 | 0.13 | 1.22 |
| (1,1359) | 1:B:157:PHE:HD2 | 1:B:160:GLU:HB2 | 3 | 1.31 | 0.13 | 1.22 |
| (1,1319) | 1:B:157:PHE:HD1 | 1:B:160:GLU:HB2 | 3 | 1.21 | 0.13 | 1.12 |
| (1,1319) | 1:B:157:PHE:HD2 | 1:B:160:GLU:HB2 | 3 | 1.21 | 0.13 | 1.12 |
| (1,845) | 1:B:185:ARG:HD2 | 1:B:186:ARG:HB2 | 3 | 0.7 | 0.13 | 0.64 |
| (1,376) | 1:B:185:ARG:HD2 | 1:B:186:ARG:HB2 | 3 | 0.5 | 0.13 | 0.44 |
| (1,108) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HG2 | 3 | 0.34 | 0.0 | 0.34 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD11 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD12 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD13 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD11 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD12 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD13 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD11 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD12 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD13 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD11 | 3 | 0.18 | 0.01 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD12 | 3 | 0.18 | 0.01 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD13 | 3 | 0.18 | 0.01 | 0.18 |
| (1,972) | 1:B:160:GLU:HA | 1:B:163:LYS:HG2 | 3 | 0.17 | 0.05 | 0.16 |
| (1,1664) | 1:B:156:ILE:H | 1:B:155:GLY:HA2 | 3 | 0.13 | 0.03 | 0.11 |
| (1,1116) | 1:B:188:THR:HB | 1:B:188:THR:HA | 3 | 0.11 | 0.0 | 0.11 |
| (1,1303) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 2 | 0.68 | 0.01 | 0.68 |
| (1,1303) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 2 | 0.68 | 0.01 | 0.68 |
| (1,390) | 1:B:185:ARG:HG2 | 1:B:186:ARG:HG3 | 2 | 0.63 | 0.45 | 0.63 |
| (1,858) | 1:B:185:ARG:HG2 | 1:B:186:ARG:HG3 | 2 | 0.63 | 0.45 | 0.63 |
| (1,1414) | 1:B:157:PHE:H | 1:B:157:PHE:HB2 | 2 | 0.61 | 0.0 | 0.61 |
| (1,1679) | 1:B:157:PHE:H | 1:B:157:PHE:HB2 | 2 | 0.61 | 0.0 | 0.61 |
| (1,1282) | 1:B:186:ARG:HA | 1:B:186:ARG:HD3 | 2 | 0.42 | 0.01 | 0.42 |
| (1,953) | 1:B:158:SER:HB2 | 1:B:155:GLY:H | 2 | 0.42 | 0.06 | 0.42 |
| (1,398) | 1:B:186:ARG:HD3 | 1:B:182:TYR:HE1 | 2 | 0.32 | 0.02 | 0.32 |
| (1,398) | 1:B:186:ARG:HD3 | 1:B:182:TYR:HE2 | 2 | 0.32 | 0.02 | 0.32 |
| (1,1094) | 1:B:186:ARG:HA | 1:B:186:ARG:HD3 | 2 | 0.22 | 0.02 | 0.22 |
| (1,83) | 1:B:162:LEU:HD21 | 1:B:166:LEU:HG | 2 | 0.18 | 0.02 | 0.18 |
| (1,83) | 1:B:162:LEU:HD22 | 1:B:166:LEU:HG | 2 | 0.18 | 0.02 | 0.18 |
| (1,83) | 1:B:162:LEU:HD23 | 1:B:166:LEU:HG | 2 | 0.18 | 0.02 | 0.18 |
| (1,1307) | 1:B:165:PHE:HA | 1:B:168:SER:HB2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG21 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG23 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG21 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG23 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG21 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG23 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD12 | 2 | 0.14 | 0.01 | 0.14 |

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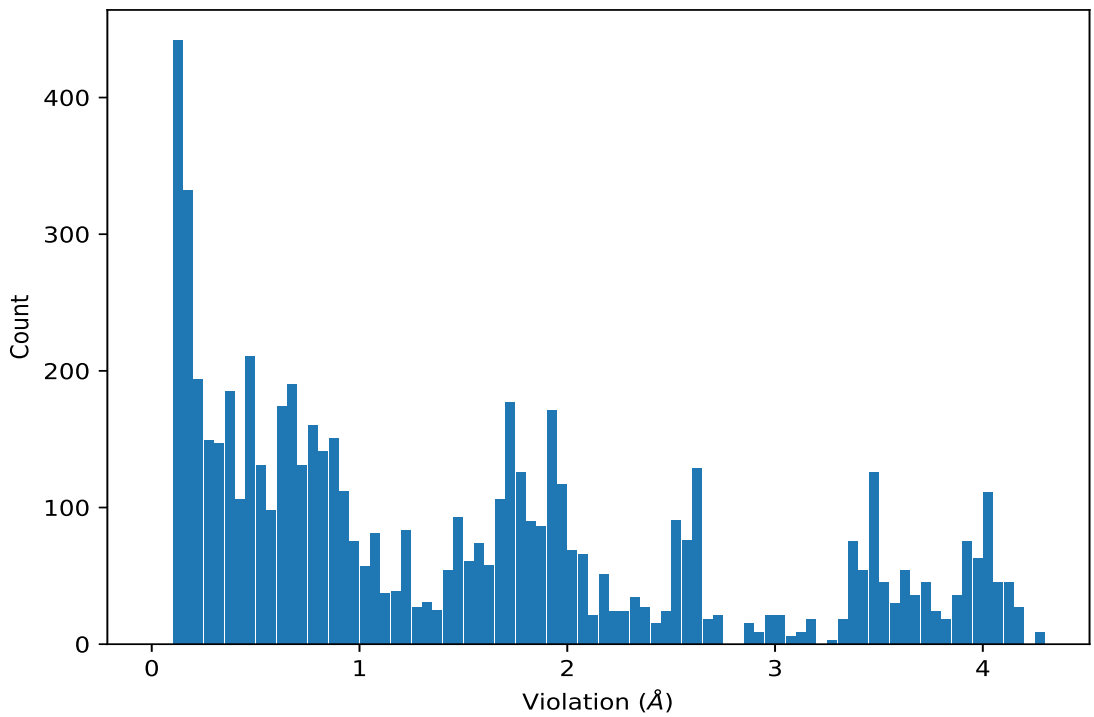
| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG21 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG23 | 2 | 0.14 | 0.01 | 0.14 |

[1]Number of violated models, [2]Standard deviation

## 9.5 All violated distance restraints (i)

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

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




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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 9 | 4.26 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 11 | 4.18 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 11 | 4.18 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 11 | 4.18 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 11 | 4.18 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 11 | 4.18 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 11 | 4.18 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 11 | 4.18 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 11 | 4.18 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 11 | 4.18 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 9 | 4.16 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 9 | 4.16 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 9 | 4.16 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 9 | 4.16 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 9 | 4.16 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 9 | 4.16 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 9 | 4.16 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 9 | 4.16 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 9 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 16 | 4.16 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 1 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 1 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 1 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 1 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 1 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 1 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 1 | 4.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 1 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 1 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 12 | 4.13 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 17 | 4.12 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 20 | 4.11 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 3 | 4.1 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 3 | 4.1 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 3 | 4.1 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 3 | 4.1 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 3 | 4.1 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 3 | 4.1 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 3 | 4.1 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 3 | 4.1 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 3 | 4.1 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 2 | 4.08 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 2 | 4.08 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 2 | 4.08 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 11 | 4.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 11 | 4.08 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 11 | 4.08 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 11 | 4.08 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 11 | 4.08 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 11 | 4.08 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 11 | 4.08 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 11 | 4.08 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 11 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 2 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 2 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 2 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 2 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 2 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 2 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 2 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 2 | 4.08 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 2 | 4.08 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 20 | 4.07 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 20 | 4.07 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 20 | 4.07 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 16 | 4.06 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 16 | 4.06 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 16 | 4.06 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 16 | 4.06 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 16 | 4.06 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 16 | 4.06 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 16 | 4.06 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 16 | 4.06 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 16 | 4.06 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 9 | 4.05 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 9 | 4.05 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 9 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 7 | 4.05 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 5 | 4.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 5 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 5 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 5 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 5 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 5 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 5 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 5 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 5 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 6 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 8 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 15 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 15 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 15 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 15 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 15 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 15 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 15 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 15 | 4.04 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 15 | 4.04 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 18 | 4.03 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 18 | 4.03 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 18 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 1 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 1 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 1 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 1 | 4.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 1 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 1 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 1 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 1 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 1 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 12 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 12 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 12 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 12 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 12 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 12 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 12 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 12 | 4.03 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 12 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 14 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 14 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 14 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 14 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 14 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 14 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 14 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 14 | 4.03 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 14 | 4.03 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 4 | 4.02 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 4 | 4.02 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 4 | 4.02 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 14 | 4.02 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 14 | 4.02 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 14 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 17 | 4.02 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 20 | 4.01 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 20 | 4.01 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 20 | 4.01 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 20 | 4.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 20 | 4.01 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 20 | 4.01 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 20 | 4.01 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 20 | 4.01 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 20 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 18 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 18 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 18 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 18 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 18 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 18 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 18 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 18 | 4.01 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 18 | 4.01 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 11 | 4.0 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 11 | 4.0 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 11 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 3 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 3 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 3 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 3 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 3 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 3 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 3 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 3 | 4.0 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 3 | 4.0 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 8 | 3.99 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 8 | 3.99 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 8 | 3.99 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 15 | 3.99 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 15 | 3.99 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 15 | 3.99 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 6 | 3.98 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 6 | 3.98 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 6 | 3.98 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 2 | 3.98 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 2 | 3.98 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 2 | 3.98 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 2 | 3.98 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 2 | 3.98 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 2 | 3.98 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 2 | 3.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 2 | 3.98 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 2 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 19 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 19 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 19 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 19 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 19 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 19 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 19 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 19 | 3.98 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 19 | 3.98 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 3 | 3.97 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 3 | 3.97 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 3 | 3.97 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 9 | 3.97 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 9 | 3.97 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 9 | 3.97 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 13 | 3.97 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 13 | 3.97 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 13 | 3.97 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 11 | 3.97 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 11 | 3.97 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 11 | 3.97 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 9 | 3.95 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 9 | 3.95 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 9 | 3.95 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 17 | 3.95 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 17 | 3.95 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 17 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 7 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 7 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 7 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 7 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 7 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 7 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 7 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 7 | 3.95 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 7 | 3.95 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 13 | 3.95 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 13 | 3.95 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 13 | 3.95 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 13 | 3.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 13 | 3.95 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 13 | 3.95 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 13 | 3.95 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 13 | 3.95 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 13 | 3.95 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 20 | 3.94 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 20 | 3.94 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 20 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 5 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 6 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 8 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 15 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 15 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 15 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 15 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 15 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 15 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 15 | 3.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 15 | 3.94 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 15 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 10 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 10 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 10 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 10 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 10 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 10 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 10 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 10 | 3.94 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 10 | 3.94 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 12 | 3.93 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 12 | 3.93 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 12 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 14 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 14 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 14 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 14 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 14 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 14 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 14 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 14 | 3.93 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 14 | 3.93 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 7 | 3.91 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 7 | 3.91 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 7 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 18 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 18 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 18 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 18 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 18 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 18 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 18 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 18 | 3.91 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 18 | 3.91 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 16 | 3.9 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 16 | 3.9 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 16 | 3.9 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 19 | 3.88 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 19 | 3.88 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 19 | 3.88 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 19 | 3.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 19 | 3.88 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 19 | 3.88 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 19 | 3.88 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 19 | 3.88 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 19 | 3.88 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 11 | 3.87 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 11 | 3.87 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 11 | 3.87 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 5 | 3.87 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 5 | 3.87 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 5 | 3.87 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 1 | 3.87 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 1 | 3.87 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 1 | 3.87 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 12 | 3.86 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 12 | 3.86 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 12 | 3.86 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 1 | 3.85 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 1 | 3.85 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 1 | 3.85 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 16 | 3.85 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 16 | 3.85 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 16 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 13 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 13 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 13 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 13 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 13 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 13 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 13 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 13 | 3.85 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 13 | 3.85 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 20 | 3.84 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 20 | 3.84 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 20 | 3.84 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 10 | 3.84 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 10 | 3.84 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 10 | 3.84 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 10 | 3.84 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 10 | 3.84 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 10 | 3.84 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 10 | 3.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 10 | 3.84 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 10 | 3.84 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 5 | 3.83 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 5 | 3.83 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 5 | 3.83 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 2 | 3.82 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 2 | 3.82 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 2 | 3.82 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 17 | 3.79 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 17 | 3.79 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 17 | 3.79 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 2 | 3.78 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 2 | 3.78 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 2 | 3.78 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 6 | 3.78 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 6 | 3.78 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 6 | 3.78 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 20 | 3.77 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 20 | 3.77 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 20 | 3.77 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 1 | 3.77 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 1 | 3.77 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 1 | 3.77 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 3 | 3.77 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 3 | 3.77 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 3 | 3.77 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 12 | 3.76 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 12 | 3.76 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 12 | 3.76 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 16 | 3.75 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 16 | 3.75 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 16 | 3.75 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 8 | 3.74 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 8 | 3.74 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 8 | 3.74 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 10 | 3.73 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 10 | 3.73 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 10 | 3.73 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 10 | 3.73 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 10 | 3.73 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 10 | 3.73 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 10 | 3.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 10 | 3.73 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 10 | 3.73 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 18 | 3.73 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 18 | 3.73 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 18 | 3.73 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 5 | 3.73 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 5 | 3.73 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 5 | 3.73 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 15 | 3.73 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 15 | 3.73 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 15 | 3.73 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 4 | 3.72 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 4 | 3.72 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 4 | 3.72 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 14 | 3.72 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 14 | 3.72 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 14 | 3.72 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 2 | 3.72 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 2 | 3.72 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 2 | 3.72 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 14 | 3.72 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 14 | 3.72 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 14 | 3.72 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 11 | 3.7 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 11 | 3.7 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 11 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 4 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 4 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 4 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 4 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 4 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 4 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 4 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 4 | 3.7 |
| (1,1991) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 4 | 3.7 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 8 | 3.69 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 8 | 3.69 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 8 | 3.69 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 15 | 3.69 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 15 | 3.69 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 15 | 3.69 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 17 | 3.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 17 | 3.69 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 17 | 3.69 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 6 | 3.68 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 6 | 3.68 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 6 | 3.68 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 6 | 3.68 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 6 | 3.68 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 6 | 3.68 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 3 | 3.67 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 3 | 3.67 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 3 | 3.67 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 9 | 3.67 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 9 | 3.67 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 9 | 3.67 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 13 | 3.67 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 13 | 3.67 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 13 | 3.67 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 3 | 3.67 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 3 | 3.67 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 3 | 3.67 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 17 | 3.65 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 17 | 3.65 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 17 | 3.65 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 7 | 3.65 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 7 | 3.65 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 7 | 3.65 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 10 | 3.65 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 10 | 3.65 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 10 | 3.65 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 8 | 3.64 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 8 | 3.64 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 8 | 3.64 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 13 | 3.64 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 13 | 3.64 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 13 | 3.64 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 12 | 3.63 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 12 | 3.63 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 12 | 3.63 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 15 | 3.63 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 15 | 3.63 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 15 | 3.63 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 14 | 3.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 14 | 3.62 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 14 | 3.62 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 18 | 3.62 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 18 | 3.62 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 18 | 3.62 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 7 | 3.61 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 7 | 3.61 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 7 | 3.61 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 16 | 3.6 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 16 | 3.6 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 16 | 3.6 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 19 | 3.6 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 19 | 3.6 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 19 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 4 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 4 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 4 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 4 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 4 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 4 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 4 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 4 | 3.6 |
| (1,1994) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 4 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 9 | 3.6 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 9 | 3.6 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 5 | 3.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 5 | 3.57 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 5 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 11 | 3.57 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 11 | 3.57 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 1 | 3.55 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 1 | 3.55 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 1 | 3.55 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 7 | 3.55 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 7 | 3.55 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 7 | 3.55 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 10 | 3.55 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 10 | 3.55 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 10 | 3.55 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 13 | 3.54 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 13 | 3.54 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 13 | 3.54 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 18 | 3.52 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 18 | 3.52 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 18 | 3.52 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 14 | 3.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 14 | 3.51 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 14 | 3.51 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 19 | 3.5 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 19 | 3.5 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 19 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 12 | 3.5 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 16 | 3.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 16 | 3.49 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 20 | 3.48 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 3 | 3.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 3 | 3.47 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 2 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 13 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 17 | 3.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 17 | 3.46 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 1 | 3.45 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 8 | 3.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 8 | 3.44 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 5 | 3.42 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 15 | 3.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 15 | 3.41 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 15 | 3.41 |
| (1,317) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 4 | 3.38 |
| (1,317) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 4 | 3.38 |
| (1,317) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 4 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 6 | 3.38 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 7 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 10 | 3.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 10 | 3.37 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 19 | 3.36 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 18 | 3.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 18 | 3.31 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 18 | 3.31 |
| (1,786) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG12 | 4 | 3.28 |
| (1,786) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG12 | 4 | 3.28 |
| (1,786) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG12 | 4 | 3.28 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD11 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD12 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:179:LEU:HD13 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD11 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD12 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:179:LEU:HD13 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD11 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD12 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:179:LEU:HD13 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD11 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD12 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD11 | 1:B:183:ILE:HD13 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD11 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD12 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD12 | 1:B:183:ILE:HD13 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD11 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD12 | 4 | 3.16 |
| (1,1960) | 1:B:177:ILE:HD13 | 1:B:183:ILE:HD13 | 4 | 3.16 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 18 | 3.13 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 18 | 3.13 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 18 | 3.13 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 18 | 3.13 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 18 | 3.13 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 18 | 3.13 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 18 | 3.13 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 18 | 3.13 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 18 | 3.13 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 2 | 3.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 2 | 3.08 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 2 | 3.08 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 20 | 3.07 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 20 | 3.07 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 20 | 3.07 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 8 | 3.03 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 8 | 3.03 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 8 | 3.03 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 8 | 3.03 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 8 | 3.03 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 8 | 3.03 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 8 | 3.03 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 8 | 3.03 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 8 | 3.03 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 18 | 3.03 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 18 | 3.03 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 18 | 3.03 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 4 | 3.02 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 4 | 3.02 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 4 | 3.02 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 14 | 3.02 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 14 | 3.02 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 14 | 3.02 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 11 | 3.0 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 11 | 3.0 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 11 | 3.0 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 8 | 2.99 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 8 | 2.99 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 8 | 2.99 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 15 | 2.99 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 15 | 2.99 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 15 | 2.99 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 6 | 2.98 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 6 | 2.98 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 6 | 2.98 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 3 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 3 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 3 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 9 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 9 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 9 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 13 | 2.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 13 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 13 | 2.97 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 17 | 2.95 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 17 | 2.95 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 17 | 2.95 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 12 | 2.93 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 12 | 2.93 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 12 | 2.93 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 7 | 2.91 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 7 | 2.91 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 7 | 2.91 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 16 | 2.9 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 16 | 2.9 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 16 | 2.9 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 7 | 2.89 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 7 | 2.89 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 7 | 2.89 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 7 | 2.89 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 7 | 2.89 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 7 | 2.89 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 7 | 2.89 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 7 | 2.89 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 7 | 2.89 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 5 | 2.87 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 5 | 2.87 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 5 | 2.87 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 1 | 2.85 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 1 | 2.85 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 1 | 2.85 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 9 | 2.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 9 | 2.73 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 9 | 2.73 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 19 | 2.7 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 19 | 2.7 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 19 | 2.7 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 11 | 2.66 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 11 | 2.66 |
| (1,330) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 10 | 2.63 |
| (1,330) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 10 | 2.63 |
| (1,330) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 10 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 12 | 2.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 12 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 16 | 2.63 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 1 | 2.62 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 2 | 2.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 2 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 3 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 20 | 2.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 20 | 2.61 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 17 | 2.6 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 17 | 2.6 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 9 | 2.58 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 9 | 2.58 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 9 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 5 | 2.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 5 | 2.58 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 15 | 2.57 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 6 | 2.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 6 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 8 | 2.55 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 8 | 2.55 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 19 | 2.55 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 10 | 2.54 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 7 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 18 | 2.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 18 | 2.53 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 14 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 19 | 2.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 19 | 2.52 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 10 | 2.51 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 10 | 2.51 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 2 | 2.48 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 2 | 2.48 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 2 | 2.48 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 20 | 2.47 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 20 | 2.47 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 20 | 2.47 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 13 | 2.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 13 | 2.46 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 13 | 2.46 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 18 | 2.43 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 18 | 2.43 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 18 | 2.43 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 4 | 2.42 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 4 | 2.42 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 4 | 2.42 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 14 | 2.42 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 14 | 2.42 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 14 | 2.42 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 19 | 2.4 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 19 | 2.4 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 19 | 2.4 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 11 | 2.4 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 11 | 2.4 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 11 | 2.4 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 8 | 2.39 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 8 | 2.39 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 8 | 2.39 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 15 | 2.39 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 15 | 2.39 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 15 | 2.39 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 9 | 2.38 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 9 | 2.38 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 9 | 2.38 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 6 | 2.38 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 6 | 2.38 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 6 | 2.38 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 3 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 3 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 3 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 9 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 9 | 2.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 9 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 13 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 13 | 2.37 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 13 | 2.37 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 15 | 2.36 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 15 | 2.36 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 15 | 2.36 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 17 | 2.35 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 17 | 2.35 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 17 | 2.35 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 15 | 2.34 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 15 | 2.34 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 15 | 2.34 |
| (1,800) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 10 | 2.33 |
| (1,800) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 10 | 2.33 |
| (1,800) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 10 | 2.33 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 12 | 2.33 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 12 | 2.33 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 12 | 2.33 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 7 | 2.31 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 7 | 2.31 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 7 | 2.31 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 16 | 2.3 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 16 | 2.3 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 16 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD11 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD12 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HD13 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD11 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD12 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HD13 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD11 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD12 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HD13 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG21 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG22 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD11 | 1:B:177:ILE:HG23 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG21 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG22 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD12 | 1:B:177:ILE:HG23 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG21 | 4 | 2.3 |
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG22 | 4 | 2.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1963) | 1:B:179:LEU:HD13 | 1:B:177:ILE:HG23 | 4 | 2.3 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 10 | 2.3 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 6 | 2.29 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 6 | 2.29 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 6 | 2.29 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 2 | 2.28 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 2 | 2.28 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 2 | 2.28 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 19 | 2.28 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 19 | 2.28 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 19 | 2.28 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 10 | 2.27 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 10 | 2.27 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 10 | 2.27 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 5 | 2.27 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 5 | 2.27 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 5 | 2.27 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 14 | 2.27 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 14 | 2.27 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 14 | 2.27 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 20 | 2.26 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 20 | 2.26 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 20 | 2.26 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 1 | 2.25 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 1 | 2.25 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 1 | 2.25 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 3 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 3 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 3 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 4 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 4 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 4 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 8 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 8 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 8 | 2.24 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 2 | 2.23 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 2 | 2.23 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 2 | 2.23 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 18 | 2.23 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 18 | 2.23 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 18 | 2.23 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 11 | 2.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 11 | 2.22 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 11 | 2.22 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 12 | 2.21 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 12 | 2.21 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 12 | 2.21 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 5 | 2.2 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 5 | 2.2 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 5 | 2.2 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 13 | 2.19 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 13 | 2.19 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 13 | 2.19 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 20 | 2.18 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 20 | 2.18 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 20 | 2.18 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 19 | 2.18 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 19 | 2.18 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 19 | 2.18 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 1 | 2.18 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 1 | 2.18 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 1 | 2.18 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 9 | 2.18 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 9 | 2.18 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 9 | 2.18 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 10 | 2.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 10 | 2.17 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 10 | 2.17 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 9 | 2.16 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 9 | 2.16 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 9 | 2.16 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 17 | 2.16 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 17 | 2.16 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 17 | 2.16 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 8 | 2.15 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 8 | 2.15 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 8 | 2.15 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 11 | 2.14 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 11 | 2.14 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 11 | 2.14 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 16 | 2.14 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 16 | 2.14 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 16 | 2.14 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 12 | 2.13 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 12 | 2.13 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 12 | 2.13 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 7 | 2.12 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 7 | 2.12 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 7 | 2.12 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 4 | 2.11 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 4 | 2.11 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 4 | 2.11 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 14 | 2.11 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 14 | 2.11 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 14 | 2.11 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 16 | 2.1 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 16 | 2.1 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 16 | 2.1 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 13 | 2.09 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 13 | 2.09 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 13 | 2.09 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 18 | 2.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 18 | 2.08 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 18 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 2 | 2.08 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 2 | 2.08 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 17 | 2.07 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 17 | 2.07 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 17 | 2.07 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 3 | 2.06 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 3 | 2.06 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 3 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 8 | 2.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 8 | 2.06 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 8 | 2.06 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 6 | 2.04 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 6 | 2.04 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 6 | 2.04 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 8 | 2.04 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 8 | 2.04 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 8 | 2.04 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 20 | 2.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 20 | 2.03 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 19 | 2.02 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 19 | 2.02 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 10 | 2.01 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 10 | 2.01 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 10 | 2.01 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 10 | 2.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 10 | 2.01 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 10 | 2.01 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 5 | 2.0 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 5 | 2.0 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 5 | 2.0 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 11 | 1.99 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 11 | 1.99 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 1 | 1.98 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 1 | 1.98 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 1 | 1.98 |
| (1,804) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 7 | 1.98 |
| (1,804) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 7 | 1.98 |
| (1,804) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 7 | 1.98 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 19 | 1.98 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 19 | 1.98 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 19 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 12 | 1.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 12 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 15 | 1.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 15 | 1.98 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 15 | 1.98 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 10 | 1.97 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 10 | 1.97 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 4 | 1.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 4 | 1.94 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 9 | 1.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 9 | 1.93 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 7 | 1.92 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 7 | 1.92 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 4 | 1.91 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 4 | 1.91 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 4 | 1.91 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 4 | 1.91 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 4 | 1.91 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 4 | 1.91 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 4 | 1.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 4 | 1.91 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 4 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 1 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 6 | 1.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 6 | 1.91 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 17 | 1.9 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 17 | 1.9 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 15 | 1.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 15 | 1.89 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 15 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 3 | 1.89 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 3 | 1.89 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 2 | 1.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 2 | 1.88 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 2 | 1.88 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 13 | 1.87 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 8 | 1.86 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 8 | 1.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 6 | 1.85 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 8 | 1.84 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 8 | 1.84 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 8 | 1.84 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 15 | 1.84 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 15 | 1.84 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 15 | 1.84 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 20 | 1.83 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 19 | 1.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 19 | 1.82 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 19 | 1.82 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 14 | 1.81 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 14 | 1.81 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 14 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 13 | 1.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 13 | 1.81 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 13 | 1.81 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 11 | 1.79 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 11 | 1.79 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 14 | 1.79 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 4 | 1.78 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 4 | 1.78 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 4 | 1.78 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 2 | 1.78 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 2 | 1.78 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 2 | 1.78 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 19 | 1.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 19 | 1.78 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 19 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 16 | 1.78 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 16 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 12 | 1.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 12 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 15 | 1.78 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 15 | 1.78 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 10 | 1.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 10 | 1.77 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 10 | 1.77 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 19 | 1.76 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 19 | 1.76 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 19 | 1.76 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 2 | 1.76 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 11 | 1.75 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 10 | 1.74 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 10 | 1.74 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 10 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 4 | 1.74 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 9 | 1.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 9 | 1.73 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 9 | 1.73 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 2 | 1.72 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 2 | 1.72 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 2 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 7 | 1.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 7 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 7 | 1.72 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 20 | 1.72 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 7 | 1.72 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 18 | 1.72 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 1 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 6 | 1.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 6 | 1.71 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 6 | 1.71 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 15 | 1.7 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 15 | 1.7 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 15 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 17 | 1.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 17 | 1.7 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 17 | 1.7 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 19 | 1.7 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 19 | 1.7 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 19 | 1.7 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 15 | 1.69 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 15 | 1.69 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 15 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 5 | 1.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 5 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 14 | 1.69 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 14 | 1.69 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 15 | 1.69 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 15 | 1.69 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 15 | 1.69 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 15 | 1.69 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 15 | 1.69 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 15 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 3 | 1.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 3 | 1.69 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 3 | 1.69 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 20 | 1.68 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 20 | 1.68 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 20 | 1.68 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 2 | 1.68 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 2 | 1.67 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 2 | 1.67 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 2 | 1.67 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 2 | 1.67 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 2 | 1.67 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 2 | 1.67 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 9 | 1.66 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 9 | 1.66 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 9 | 1.66 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 8 | 1.65 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 8 | 1.65 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 8 | 1.65 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 11 | 1.64 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 11 | 1.64 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 11 | 1.64 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 12 | 1.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 12 | 1.63 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 12 | 1.63 |
| (1,1959) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 10 | 1.63 |
| (1,1959) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 10 | 1.63 |
| (1,1959) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 10 | 1.63 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 18 | 1.61 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 18 | 1.61 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 18 | 1.61 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 18 | 1.61 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 18 | 1.61 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 18 | 1.61 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 4 | 1.61 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 4 | 1.61 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 4 | 1.61 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 14 | 1.61 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 14 | 1.61 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 14 | 1.61 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 14 | 1.61 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 14 | 1.61 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 14 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 13 | 1.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 13 | 1.61 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 13 | 1.61 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 16 | 1.6 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 16 | 1.6 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 16 | 1.6 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 15 | 1.6 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 15 | 1.6 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 15 | 1.6 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 18 | 1.6 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 13 | 1.59 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 13 | 1.59 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 13 | 1.59 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 20 | 1.59 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 20 | 1.59 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 20 | 1.59 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 20 | 1.59 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 20 | 1.59 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 20 | 1.59 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 18 | 1.58 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 18 | 1.58 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 18 | 1.58 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 4 | 1.58 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 4 | 1.58 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 4 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 16 | 1.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 16 | 1.58 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 16 | 1.58 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 6 | 1.57 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 6 | 1.57 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 6 | 1.57 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 17 | 1.57 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 17 | 1.57 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 17 | 1.57 |
| (1,846) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 2 | 1.56 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 3 | 1.56 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 3 | 1.56 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 3 | 1.56 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 19 | 1.56 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 19 | 1.56 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 19 | 1.56 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 9 | 1.56 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 9 | 1.56 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 9 | 1.56 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 9 | 1.56 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 9 | 1.56 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 9 | 1.56 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 19 | 1.56 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 8 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 8 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 8 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 8 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 8 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 8 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 11 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 11 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 11 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 11 | 1.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 11 | 1.55 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 11 | 1.55 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 8 | 1.54 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 8 | 1.54 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 8 | 1.54 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 8 | 1.54 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 8 | 1.54 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 8 | 1.54 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 6 | 1.54 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 6 | 1.54 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 6 | 1.54 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 10 | 1.54 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 10 | 1.54 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 10 | 1.54 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 4 | 1.54 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 4 | 1.54 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 4 | 1.54 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 4 | 1.54 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 4 | 1.54 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 4 | 1.54 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 12 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 12 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 12 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 12 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 12 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 12 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 14 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 14 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 14 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 14 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 14 | 1.53 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 14 | 1.53 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 2 | 1.52 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 2 | 1.52 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 2 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 18 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 18 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 18 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 18 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 18 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 18 | 1.52 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 13 | 1.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 13 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 13 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 13 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 13 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 13 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 16 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 16 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 16 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 16 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 16 | 1.51 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 16 | 1.51 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 5 | 1.5 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 5 | 1.5 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 5 | 1.5 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 7 | 1.5 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 7 | 1.5 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 7 | 1.5 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 5 | 1.5 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 5 | 1.5 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 5 | 1.5 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 19 | 1.5 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 17 | 1.49 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 17 | 1.49 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 17 | 1.49 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 17 | 1.49 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 17 | 1.49 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 17 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 5 | 1.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 5 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 14 | 1.49 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 14 | 1.49 |
| (1,1359) | 1:B:157:PHE:HD1 | 1:B:160:GLU:HB2 | 14 | 1.49 |
| (1,1359) | 1:B:157:PHE:HD2 | 1:B:160:GLU:HB2 | 14 | 1.49 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 13 | 1.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 13 | 1.48 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 13 | 1.48 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 1 | 1.48 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 1 | 1.48 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 1 | 1.48 |
| (1,335) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HB | 7 | 1.48 |
| (1,335) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HB | 7 | 1.48 |
| (1,335) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HB | 7 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 3 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 3 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 3 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 3 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 3 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 3 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 6 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 6 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 6 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 6 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 6 | 1.48 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 6 | 1.48 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 19 | 1.46 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 19 | 1.46 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 19 | 1.46 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 4 | 1.46 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 20 | 1.45 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 20 | 1.45 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 20 | 1.45 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 10 | 1.45 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 10 | 1.45 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 10 | 1.45 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 1 | 1.43 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 1 | 1.43 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 1 | 1.43 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 15 | 1.43 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 15 | 1.43 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 15 | 1.43 |
| (1,846) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 7 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 5 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 5 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 5 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 5 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 5 | 1.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 5 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 7 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 7 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 7 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 7 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 7 | 1.42 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 7 | 1.42 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 8 | 1.42 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 18 | 1.41 |
| (1,1992) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 18 | 1.41 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 1 | 1.41 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 1 | 1.41 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 1 | 1.41 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 1 | 1.41 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 1 | 1.41 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 1 | 1.41 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 20 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1319) | 1:B:157:PHE:HD1 | 1:B:160:GLU:HB2 | 14 | 1.39 |
| (1,1319) | 1:B:157:PHE:HD2 | 1:B:160:GLU:HB2 | 14 | 1.39 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 7 | 1.38 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 7 | 1.38 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 7 | 1.38 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 7 | 1.38 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 7 | 1.38 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 7 | 1.38 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 12 | 1.38 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 12 | 1.38 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 12 | 1.38 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 6 | 1.38 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 6 | 1.37 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 6 | 1.37 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 6 | 1.37 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 8 | 1.37 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 17 | 1.36 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 17 | 1.36 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 17 | 1.36 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 19 | 1.36 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 19 | 1.36 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 19 | 1.36 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 10 | 1.35 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 10 | 1.35 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 10 | 1.35 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 2 | 1.34 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 2 | 1.34 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 2 | 1.34 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 10 | 1.34 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 10 | 1.34 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 10 | 1.34 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 10 | 1.34 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 10 | 1.34 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 10 | 1.34 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 14 | 1.33 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 14 | 1.33 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 14 | 1.33 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 20 | 1.33 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 20 | 1.33 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 20 | 1.33 |
| (1,437) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 10 | 1.32 |
| (1,437) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 10 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,437) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 10 | 1.32 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 12 | 1.31 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 12 | 1.31 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 12 | 1.31 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 10 | 1.3 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 5 | 1.3 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 5 | 1.3 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 5 | 1.3 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 7 | 1.3 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 7 | 1.3 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 7 | 1.3 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 1 | 1.3 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 1 | 1.3 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 3 | 1.3 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 4 | 1.29 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 4 | 1.29 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 4 | 1.29 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 13 | 1.28 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 13 | 1.28 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 13 | 1.28 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 11 | 1.28 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 11 | 1.28 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 11 | 1.28 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 18 | 1.27 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 18 | 1.27 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 18 | 1.27 |
| (1,377) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 2 | 1.26 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 6 | 1.26 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 6 | 1.26 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 6 | 1.26 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 8 | 1.26 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 8 | 1.26 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 8 | 1.26 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 3 | 1.26 |
| (1,846) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 13 | 1.25 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 20 | 1.25 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 20 | 1.25 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 20 | 1.25 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 3 | 1.25 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 3 | 1.25 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 3 | 1.25 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 9 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 9 | 1.24 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 9 | 1.24 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 2 | 1.24 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 2 | 1.24 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 2 | 1.24 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 19 | 1.24 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 19 | 1.24 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 19 | 1.24 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 19 | 1.24 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 19 | 1.24 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 19 | 1.24 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 10 | 1.23 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 10 | 1.23 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 10 | 1.23 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 10 | 1.23 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 10 | 1.23 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 10 | 1.23 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 10 | 1.23 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 10 | 1.23 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 10 | 1.23 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 15 | 1.23 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 15 | 1.23 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 15 | 1.23 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 1 | 1.23 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 1 | 1.23 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 1 | 1.23 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 19 | 1.23 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 19 | 1.23 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 19 | 1.23 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 19 | 1.23 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 19 | 1.23 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 19 | 1.23 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 16 | 1.23 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 16 | 1.23 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 16 | 1.23 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 14 | 1.23 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 14 | 1.23 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 14 | 1.23 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 20 | 1.23 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 20 | 1.23 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 20 | 1.23 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 3 | 1.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 3 | 1.22 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 3 | 1.22 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 13 | 1.22 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 13 | 1.22 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 13 | 1.22 |
| (1,1359) | 1:B:157:PHE:HD1 | 1:B:160:GLU:HB2 | 13 | 1.22 |
| (1,1359) | 1:B:157:PHE:HD2 | 1:B:160:GLU:HB2 | 13 | 1.22 |
| (1,1359) | 1:B:157:PHE:HD1 | 1:B:160:GLU:HB2 | 19 | 1.22 |
| (1,1359) | 1:B:157:PHE:HD2 | 1:B:160:GLU:HB2 | 19 | 1.22 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG21 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG22 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HG23 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG21 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG22 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HG23 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG21 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG22 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HG23 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD11 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD12 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:187:LEU:HD13 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD11 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD12 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:187:LEU:HD13 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD11 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD12 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:187:LEU:HD13 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD11 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD12 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG21 | 1:B:183:ILE:HD13 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD11 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD12 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG22 | 1:B:183:ILE:HD13 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD11 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD12 | 18 | 1.21 |
| (1,1961) | 1:B:181:ILE:HG23 | 1:B:183:ILE:HD13 | 18 | 1.21 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 12 | 1.21 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 12 | 1.21 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 12 | 1.21 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 16 | 1.21 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 10 | 1.19 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 10 | 1.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 10 | 1.19 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 10 | 1.19 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 10 | 1.19 |
| (1,1987) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 10 | 1.19 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 4 | 1.19 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 4 | 1.19 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 4 | 1.19 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 14 | 1.19 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 12 | 1.18 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 12 | 1.18 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 12 | 1.18 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 11 | 1.18 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 11 | 1.18 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 11 | 1.18 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 10 | 1.17 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 17 | 1.16 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 17 | 1.16 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 17 | 1.16 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 1 | 1.16 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 1 | 1.16 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 1 | 1.16 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 5 | 1.16 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 5 | 1.16 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 5 | 1.16 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 6 | 1.16 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 6 | 1.16 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 6 | 1.16 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 8 | 1.16 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 8 | 1.16 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 8 | 1.16 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 2 | 1.16 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 16 | 1.15 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 16 | 1.15 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 16 | 1.15 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 3 | 1.15 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 3 | 1.15 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 3 | 1.15 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 3 | 1.14 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 3 | 1.14 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 3 | 1.14 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 10 | 1.14 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 10 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 10 | 1.14 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 9 | 1.14 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 9 | 1.14 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 9 | 1.14 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 16 | 1.13 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 16 | 1.13 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 16 | 1.13 |
| (1,377) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 7 | 1.12 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 17 | 1.12 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 17 | 1.12 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 17 | 1.12 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 13 | 1.12 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 13 | 1.12 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 13 | 1.12 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 7 | 1.12 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 7 | 1.12 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 7 | 1.12 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 20 | 1.12 |
| (1,1319) | 1:B:157:PHE:HD1 | 1:B:160:GLU:HB2 | 13 | 1.12 |
| (1,1319) | 1:B:157:PHE:HD2 | 1:B:160:GLU:HB2 | 13 | 1.12 |
| (1,1319) | 1:B:157:PHE:HD1 | 1:B:160:GLU:HB2 | 19 | 1.12 |
| (1,1319) | 1:B:157:PHE:HD2 | 1:B:160:GLU:HB2 | 19 | 1.12 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 13 | 1.11 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 13 | 1.11 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 13 | 1.11 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 14 | 1.11 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 19 | 1.1 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 19 | 1.1 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 19 | 1.1 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 14 | 1.1 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 14 | 1.1 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 14 | 1.1 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 18 | 1.09 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 18 | 1.09 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 18 | 1.09 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 15 | 1.09 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 15 | 1.09 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 15 | 1.09 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 15 | 1.09 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 15 | 1.09 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 15 | 1.09 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 18 | 1.09 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 18 | 1.09 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 18 | 1.09 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 19 | 1.09 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 19 | 1.09 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 19 | 1.09 |
| (1,858) | 1:B:185:ARG:HG2 | 1:B:186:ARG:HG3 | 11 | 1.08 |
| (1,390) | 1:B:185:ARG:HG2 | 1:B:186:ARG:HG3 | 11 | 1.08 |
| (1,1981) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 7 | 1.08 |
| (1,1981) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 7 | 1.08 |
| (1,1981) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 7 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 3 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 3 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 3 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 9 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 9 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 9 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 11 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 11 | 1.08 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 11 | 1.08 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 18 | 1.07 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 18 | 1.07 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 18 | 1.07 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 2 | 1.07 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 2 | 1.07 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 2 | 1.07 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 2 | 1.07 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 2 | 1.07 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 2 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 6 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 6 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 6 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 10 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 10 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 10 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 15 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 15 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 15 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 16 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 16 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 16 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 17 | 1.07 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 17 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 17 | 1.07 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 9 | 1.07 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 1 | 1.06 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 1 | 1.06 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 1 | 1.06 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 5 | 1.06 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 5 | 1.06 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 5 | 1.06 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 2 | 1.06 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 2 | 1.06 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 2 | 1.06 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 4 | 1.06 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 4 | 1.06 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 4 | 1.06 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 1 | 1.05 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 1 | 1.05 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 1 | 1.05 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 5 | 1.05 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 5 | 1.05 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 5 | 1.05 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 8 | 1.05 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 8 | 1.05 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 8 | 1.05 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 16 | 1.05 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 16 | 1.05 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 16 | 1.05 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 16 | 1.05 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 16 | 1.05 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 16 | 1.05 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 19 | 1.04 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 19 | 1.04 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 19 | 1.04 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 12 | 1.04 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 12 | 1.04 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 12 | 1.04 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 18 | 1.04 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 18 | 1.04 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 18 | 1.04 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 18 | 1.04 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 18 | 1.04 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 18 | 1.04 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 10 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 10 | 1.03 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 10 | 1.03 |
| (1,1990) | 1:B:181:ILE:HD11 | 1:B:183:ILE:HB | 10 | 1.03 |
| (1,1990) | 1:B:181:ILE:HD12 | 1:B:183:ILE:HB | 10 | 1.03 |
| (1,1990) | 1:B:181:ILE:HD13 | 1:B:183:ILE:HB | 10 | 1.03 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 10 | 1.03 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 10 | 1.03 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 10 | 1.03 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 2 | 1.03 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 2 | 1.03 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 2 | 1.03 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 14 | 1.03 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 14 | 1.03 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 14 | 1.03 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 2 | 1.03 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 2 | 1.03 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 2 | 1.03 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 14 | 1.03 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 14 | 1.03 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 14 | 1.03 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 3 | 1.02 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 3 | 1.02 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 3 | 1.02 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 17 | 1.02 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 17 | 1.02 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 17 | 1.02 |
| (1,1941) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 20 | 1.02 |
| (1,1941) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 20 | 1.02 |
| (1,1941) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 20 | 1.02 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 3 | 1.02 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 3 | 1.02 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 3 | 1.02 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 3 | 1.02 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 3 | 1.02 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 3 | 1.02 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 10 | 1.01 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 10 | 1.01 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 10 | 1.01 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 10 | 1.01 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 10 | 1.01 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 10 | 1.01 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 5 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 15 | 1.0 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 18 | 1.0 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 20 | 0.99 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 20 | 0.99 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 20 | 0.99 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 20 | 0.99 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 20 | 0.99 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 20 | 0.99 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 18 | 0.99 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 18 | 0.99 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 18 | 0.99 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 6 | 0.98 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 6 | 0.98 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 6 | 0.98 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 6 | 0.98 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 6 | 0.98 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 6 | 0.98 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 6 | 0.98 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 6 | 0.98 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 6 | 0.98 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 2 | 0.98 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 2 | 0.98 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 2 | 0.98 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 3 | 0.98 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 3 | 0.98 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 3 | 0.98 |
| (1,1949) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA2 | 7 | 0.98 |
| (1,1949) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA2 | 7 | 0.98 |
| (1,1949) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA2 | 7 | 0.98 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 2 | 0.98 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 2 | 0.98 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 2 | 0.98 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 3 | 0.98 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 3 | 0.98 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 3 | 0.98 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 8 | 0.98 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 8 | 0.98 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 8 | 0.98 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 8 | 0.98 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 8 | 0.98 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 8 | 0.98 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 13 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 15 | 0.97 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 9 | 0.96 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 9 | 0.96 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 9 | 0.96 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 9 | 0.96 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 9 | 0.96 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 9 | 0.96 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 19 | 0.96 |
| (1,1159) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 15 | 0.96 |
| (1,377) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 13 | 0.95 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 5 | 0.95 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 5 | 0.95 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 5 | 0.95 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 3 | 0.95 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 3 | 0.95 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 3 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 8 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 8 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 8 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 8 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 8 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 8 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 11 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 11 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 11 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 11 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 11 | 0.95 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 11 | 0.95 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 3 | 0.95 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 3 | 0.95 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 3 | 0.95 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 5 | 0.95 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 5 | 0.95 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 5 | 0.95 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 4 | 0.95 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 8 | 0.94 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 8 | 0.94 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 8 | 0.94 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 15 | 0.94 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 15 | 0.94 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 15 | 0.94 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 3 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 3 | 0.94 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 3 | 0.94 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 4 | 0.94 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 4 | 0.94 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 4 | 0.94 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 4 | 0.94 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 4 | 0.94 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 4 | 0.94 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 15 | 0.94 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 15 | 0.94 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 15 | 0.94 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 17 | 0.94 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 18 | 0.93 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 18 | 0.93 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 18 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 12 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 12 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 12 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 12 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 12 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 12 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 14 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 14 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 14 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 14 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 14 | 0.93 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 14 | 0.93 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 18 | 0.93 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 18 | 0.93 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 18 | 0.93 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 20 | 0.93 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 20 | 0.93 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 20 | 0.93 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 20 | 0.93 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 20 | 0.93 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 20 | 0.93 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 16 | 0.92 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 16 | 0.92 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 16 | 0.92 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 4 | 0.92 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 4 | 0.92 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 4 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 11 | 0.92 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 11 | 0.92 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 11 | 0.92 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 2 | 0.92 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 2 | 0.92 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 2 | 0.92 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 12 | 0.92 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 12 | 0.92 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 12 | 0.92 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 7 | 0.92 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 7 | 0.92 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 7 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 18 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 18 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 18 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 18 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 18 | 0.92 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 18 | 0.92 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 2 | 0.92 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 2 | 0.92 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 2 | 0.92 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 12 | 0.92 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 12 | 0.92 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 12 | 0.92 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 4 | 0.92 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 4 | 0.92 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 4 | 0.92 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 11 | 0.92 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 11 | 0.92 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 11 | 0.92 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 11 | 0.91 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 11 | 0.91 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 11 | 0.91 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 5 | 0.91 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 5 | 0.91 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 5 | 0.91 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 13 | 0.91 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 13 | 0.91 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 13 | 0.91 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 13 | 0.91 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 13 | 0.91 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 13 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 13 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 13 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 13 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 13 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 13 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 13 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 16 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 16 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 16 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 16 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 16 | 0.91 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 16 | 0.91 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 5 | 0.91 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 5 | 0.91 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 5 | 0.91 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 13 | 0.91 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 13 | 0.91 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 13 | 0.91 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 14 | 0.9 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 14 | 0.9 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 14 | 0.9 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 13 | 0.89 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 13 | 0.89 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 13 | 0.89 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 19 | 0.89 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 19 | 0.89 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 19 | 0.89 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 6 | 0.89 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 6 | 0.89 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 6 | 0.89 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 18 | 0.89 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 18 | 0.89 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 18 | 0.89 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 19 | 0.89 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 19 | 0.89 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 19 | 0.89 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 17 | 0.89 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 17 | 0.89 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 17 | 0.89 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 17 | 0.89 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 17 | 0.89 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 17 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 14 | 0.89 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 6 | 0.89 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 6 | 0.89 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 6 | 0.89 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 13 | 0.89 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 13 | 0.89 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 13 | 0.89 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 19 | 0.89 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 19 | 0.89 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 19 | 0.89 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 11 | 0.89 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 11 | 0.89 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 11 | 0.89 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 13 | 0.89 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 13 | 0.89 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 13 | 0.89 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 11 | 0.89 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 11 | 0.89 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 11 | 0.89 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 13 | 0.89 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 13 | 0.89 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 13 | 0.89 |
| (1,845) | 1:B:185:ARG:HD2 | 1:B:186:ARG:HB2 | 2 | 0.88 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 15 | 0.88 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 15 | 0.88 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 15 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 3 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 3 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 3 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 9 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 9 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 9 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 11 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 11 | 0.88 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 11 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 3 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 3 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 3 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 3 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 3 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 3 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 6 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 6 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 6 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 6 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 6 | 0.88 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 6 | 0.88 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 15 | 0.88 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 15 | 0.88 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 15 | 0.88 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 13 | 0.87 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 1 | 0.87 |
| (1,437) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 18 | 0.87 |
| (1,437) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 18 | 0.87 |
| (1,437) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 18 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 6 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 6 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 6 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 10 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 10 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 10 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 15 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 15 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 15 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 16 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 16 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 16 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 17 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 17 | 0.87 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 17 | 0.87 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 10 | 0.87 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 18 | 0.87 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 13 | 0.86 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 13 | 0.86 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 13 | 0.86 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 9 | 0.86 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 9 | 0.86 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 9 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 11 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 11 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 11 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 14 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 14 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 14 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 19 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 19 | 0.86 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 19 | 0.86 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 2 | 0.86 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 2 | 0.86 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 2 | 0.86 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 4 | 0.86 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 4 | 0.86 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 4 | 0.86 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 6 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 11 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 11 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 11 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 14 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 14 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 14 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 19 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 19 | 0.86 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 19 | 0.86 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 9 | 0.86 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 9 | 0.86 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 9 | 0.86 |
| (1,1691) | 1:B:158:SER:H | 1:B:162:LEU:HG | 7 | 0.86 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 20 | 0.86 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 6 | 0.85 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 20 | 0.85 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 20 | 0.85 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 20 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 1 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 1 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 1 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 5 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 5 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 5 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 8 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 8 | 0.85 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 8 | 0.85 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 16 | 0.85 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 16 | 0.85 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 16 | 0.85 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 20 | 0.85 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 20 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 20 | 0.85 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 4 | 0.85 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 6 | 0.85 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 7 | 0.85 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 1 | 0.84 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 1 | 0.84 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 1 | 0.84 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 9 | 0.84 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 9 | 0.84 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 9 | 0.84 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 12 | 0.84 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 12 | 0.84 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 12 | 0.84 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 18 | 0.84 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 18 | 0.84 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 18 | 0.84 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 1 | 0.84 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 1 | 0.84 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 1 | 0.84 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 9 | 0.84 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 9 | 0.84 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 9 | 0.84 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 17 | 0.84 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 13 | 0.84 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 10 | 0.83 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 10 | 0.83 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 10 | 0.83 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 8 | 0.83 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 8 | 0.83 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 8 | 0.83 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 12 | 0.83 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 12 | 0.83 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 12 | 0.83 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 14 | 0.83 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 14 | 0.83 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 14 | 0.83 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 8 | 0.83 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 8 | 0.83 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 8 | 0.83 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 10 | 0.83 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 10 | 0.83 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 10 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 2 | 0.83 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 2 | 0.83 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 2 | 0.83 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 14 | 0.83 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 14 | 0.83 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 14 | 0.83 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 8 | 0.83 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 8 | 0.83 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 8 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 8 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 8 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 8 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 12 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 12 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 12 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 14 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 14 | 0.83 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 14 | 0.83 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 2 | 0.83 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 14 | 0.83 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 1 | 0.82 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 1 | 0.82 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 1 | 0.82 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 1 | 0.82 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 1 | 0.82 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 1 | 0.82 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 11 | 0.82 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 11 | 0.82 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 11 | 0.82 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 17 | 0.82 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 17 | 0.82 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 17 | 0.82 |
| (1,1973) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 20 | 0.82 |
| (1,1973) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 20 | 0.82 |
| (1,1973) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 20 | 0.82 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 3 | 0.82 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 3 | 0.82 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 3 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 5 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 5 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 5 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 5 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 5 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 5 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 7 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 7 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 7 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 7 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 7 | 0.82 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 7 | 0.82 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 17 | 0.82 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 17 | 0.82 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 17 | 0.82 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 17 | 0.82 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 17 | 0.82 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 17 | 0.82 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 20 | 0.82 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 20 | 0.82 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 20 | 0.82 |
| (1,1698) | 1:B:160:GLU:H | 1:B:158:SER:HB2 | 16 | 0.82 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 17 | 0.82 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 17 | 0.82 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 17 | 0.82 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 20 | 0.82 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 20 | 0.82 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 20 | 0.82 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 8 | 0.82 |
| (2,30) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 13 | 0.81 |
| (2,26) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 13 | 0.81 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 9 | 0.81 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 9 | 0.81 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 9 | 0.81 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 6 | 0.81 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 6 | 0.81 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 6 | 0.81 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 1 | 0.81 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 1 | 0.81 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 1 | 0.81 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 1 | 0.81 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 1 | 0.81 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 1 | 0.81 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 3 | 0.81 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 13 | 0.81 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 6 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 6 | 0.81 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 6 | 0.81 |
| (1,1691) | 1:B:158:SER:H | 1:B:162:LEU:HG | 12 | 0.81 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 15 | 0.81 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 3 | 0.81 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 11 | 0.81 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 12 | 0.81 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 16 | 0.81 |
| (1,437) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 8 | 0.8 |
| (1,437) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 8 | 0.8 |
| (1,437) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 8 | 0.8 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 17 | 0.8 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 17 | 0.8 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 17 | 0.8 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 17 | 0.8 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 17 | 0.8 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 17 | 0.8 |
| (1,1698) | 1:B:160:GLU:H | 1:B:158:SER:HB2 | 1 | 0.8 |
| (1,1691) | 1:B:158:SER:H | 1:B:162:LEU:HG | 15 | 0.8 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 9 | 0.79 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 9 | 0.79 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 9 | 0.79 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 4 | 0.79 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 4 | 0.79 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 4 | 0.79 |
| (1,904) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 4 | 0.79 |
| (1,904) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 4 | 0.79 |
| (1,904) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 4 | 0.79 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 20 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 1 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 2 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 4 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 5 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 6 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 7 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 8 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 9 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 10 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 12 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 13 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 14 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 18 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 19 | 0.79 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 20 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 1 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 2 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 4 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 5 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 6 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 7 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 8 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 9 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 10 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 12 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 13 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 14 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 18 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 19 | 0.79 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 20 | 0.79 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 15 | 0.79 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 2 | 0.78 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 2 | 0.78 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 2 | 0.78 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 3 | 0.78 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 3 | 0.78 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 3 | 0.78 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 2 | 0.78 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 2 | 0.78 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 2 | 0.78 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 3 | 0.78 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 3 | 0.78 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 3 | 0.78 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 8 | 0.78 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 8 | 0.78 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 8 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 1 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 1 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 1 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 7 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 7 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 7 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 12 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 12 | 0.78 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 12 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 3 | 0.78 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 11 | 0.78 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 15 | 0.78 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 16 | 0.78 |
| (1,1780) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 17 | 0.78 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 3 | 0.78 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 11 | 0.78 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 15 | 0.78 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 16 | 0.78 |
| (1,1511) | 1:B:171:LEU:H | 1:B:171:LEU:HB3 | 17 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 1 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 1 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 1 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 7 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 7 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 7 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 12 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 12 | 0.78 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 12 | 0.78 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 6 | 0.78 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 12 | 0.78 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 5 | 0.78 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 9 | 0.78 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 4 | 0.77 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 1 | 0.77 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 1 | 0.77 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 1 | 0.77 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 16 | 0.77 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 16 | 0.77 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 16 | 0.77 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 15 | 0.77 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 19 | 0.77 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 1 | 0.77 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 1 | 0.77 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 1 | 0.77 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 16 | 0.77 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 16 | 0.77 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 16 | 0.77 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 7 | 0.77 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 8 | 0.77 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 17 | 0.77 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 13 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 13 | 0.76 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 13 | 0.76 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 13 | 0.76 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 13 | 0.76 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 13 | 0.76 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 13 | 0.76 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 13 | 0.76 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 13 | 0.76 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 20 | 0.76 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 20 | 0.76 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 20 | 0.76 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 18 | 0.76 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 18 | 0.76 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 18 | 0.76 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 18 | 0.76 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 18 | 0.76 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 18 | 0.76 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 20 | 0.76 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 20 | 0.76 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 20 | 0.76 |
| (1,1425) | 1:B:158:SER:H | 1:B:162:LEU:HG | 7 | 0.76 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 13 | 0.76 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 13 | 0.76 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 13 | 0.76 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 13 | 0.76 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 13 | 0.76 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 13 | 0.76 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 11 | 0.75 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 11 | 0.75 |
| (1,903) | 1:B:188:THR:HG21 | 1:B:187:LEU:H | 18 | 0.75 |
| (1,903) | 1:B:188:THR:HG22 | 1:B:187:LEU:H | 18 | 0.75 |
| (1,903) | 1:B:188:THR:HG23 | 1:B:187:LEU:H | 18 | 0.75 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 5 | 0.75 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 5 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 5 | 0.75 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 5 | 0.75 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 5 | 0.75 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 5 | 0.75 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 1 | 0.75 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 4 | 0.75 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 11 | 0.75 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 2 | 0.75 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 2 | 0.75 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 2 | 0.75 |
| (1,1114) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 1 | 0.75 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 15 | 0.74 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 15 | 0.74 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 15 | 0.74 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 15 | 0.74 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 15 | 0.74 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 15 | 0.74 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 15 | 0.74 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 15 | 0.74 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 15 | 0.74 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 15 | 0.74 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 15 | 0.74 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 15 | 0.74 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 10 | 0.74 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 10 | 0.74 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 10 | 0.74 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 8 | 0.74 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 8 | 0.74 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 8 | 0.74 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 15 | 0.74 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 15 | 0.74 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 15 | 0.74 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 2 | 0.74 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 10 | 0.74 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 10 | 0.74 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 10 | 0.74 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 11 | 0.74 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 17 | 0.74 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 17 | 0.74 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 17 | 0.74 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 17 | 0.74 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 17 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 17 | 0.74 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 18 | 0.73 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 18 | 0.73 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 18 | 0.73 |
| (1,302) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 7 | 0.73 |
| (1,302) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 7 | 0.73 |
| (1,302) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 7 | 0.73 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 18 | 0.73 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 18 | 0.73 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 18 | 0.73 |
| (1,1943) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 7 | 0.73 |
| (1,1943) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 7 | 0.73 |
| (1,1943) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 7 | 0.73 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 4 | 0.73 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 4 | 0.73 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 4 | 0.73 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 3 | 0.73 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 3 | 0.73 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 3 | 0.73 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 4 | 0.73 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 4 | 0.73 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 4 | 0.73 |
| (1,1159) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 7 | 0.73 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 7 | 0.72 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 18 | 0.72 |
| (1,903) | 1:B:188:THR:HG21 | 1:B:187:LEU:H | 10 | 0.72 |
| (1,903) | 1:B:188:THR:HG22 | 1:B:187:LEU:H | 10 | 0.72 |
| (1,903) | 1:B:188:THR:HG23 | 1:B:187:LEU:H | 10 | 0.72 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 4 | 0.72 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 4 | 0.72 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 4 | 0.72 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 11 | 0.72 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 11 | 0.72 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 11 | 0.72 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 16 | 0.72 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 16 | 0.72 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 16 | 0.72 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 16 | 0.72 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 16 | 0.72 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 16 | 0.72 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 4 | 0.72 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 4 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 4 | 0.72 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 11 | 0.72 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 11 | 0.72 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 11 | 0.72 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 8 | 0.72 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 18 | 0.72 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 16 | 0.72 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 16 | 0.72 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 16 | 0.72 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 15 | 0.72 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 15 | 0.72 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 15 | 0.72 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 15 | 0.72 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 15 | 0.72 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 15 | 0.72 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 15 | 0.72 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 15 | 0.72 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 15 | 0.72 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 5 | 0.71 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 12 | 0.71 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 18 | 0.71 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 18 | 0.71 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 18 | 0.71 |
| (1,1425) | 1:B:158:SER:H | 1:B:162:LEU:HG | 12 | 0.71 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 8 | 0.71 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 8 | 0.71 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 8 | 0.71 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 8 | 0.71 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 8 | 0.71 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 8 | 0.71 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 14 | 0.7 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 17 | 0.7 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 5 | 0.7 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 5 | 0.7 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 5 | 0.7 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 11 | 0.7 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 11 | 0.7 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 11 | 0.7 |
| (1,1425) | 1:B:158:SER:H | 1:B:162:LEU:HG | 15 | 0.7 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 1 | 0.7 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 1 | 0.7 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 1 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 1 | 0.7 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 14 | 0.7 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 14 | 0.7 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 14 | 0.7 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 16 | 0.7 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 16 | 0.7 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 16 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 1 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 1 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 1 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 14 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 14 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 14 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 16 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 16 | 0.7 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 16 | 0.7 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 19 | 0.69 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 19 | 0.69 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 19 | 0.69 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 2 | 0.69 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 14 | 0.69 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 14 | 0.69 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 14 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 14 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 14 | 0.69 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 14 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 14 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 14 | 0.69 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 14 | 0.69 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 13 | 0.69 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 13 | 0.69 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 13 | 0.69 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 19 | 0.69 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 19 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 19 | 0.69 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 14 | 0.69 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 13 | 0.69 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 13 | 0.69 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 13 | 0.69 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 19 | 0.69 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 19 | 0.69 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 19 | 0.69 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 11 | 0.69 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 11 | 0.69 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 11 | 0.69 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 13 | 0.69 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 13 | 0.69 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 13 | 0.69 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 9 | 0.69 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 1 | 0.69 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 3 | 0.69 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 3 | 0.69 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 3 | 0.69 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 1 | 0.69 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 3 | 0.69 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 3 | 0.69 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 3 | 0.69 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 2 | 0.68 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 1 | 0.68 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 1 | 0.68 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 1 | 0.68 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 1 | 0.68 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 1 | 0.68 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 1 | 0.68 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 1 | 0.68 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 1 | 0.68 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 1 | 0.68 |
| (1,376) | 1:B:185:ARG:HD2 | 1:B:186:ARG:HB2 | 2 | 0.68 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 12 | 0.68 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 12 | 0.68 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 12 | 0.68 |
| (1,1303) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 19 | 0.68 |
| (1,1303) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 19 | 0.68 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 20 | 0.68 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 4 | 0.68 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 4 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 4 | 0.68 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 5 | 0.68 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 5 | 0.68 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 5 | 0.68 |
| (1,1159) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 13 | 0.68 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 20 | 0.68 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 4 | 0.68 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 4 | 0.68 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 4 | 0.68 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 5 | 0.68 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 5 | 0.68 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 5 | 0.68 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 6 | 0.67 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 12 | 0.67 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 19 | 0.67 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 19 | 0.67 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 19 | 0.67 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 19 | 0.67 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 19 | 0.67 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 19 | 0.67 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 19 | 0.67 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 19 | 0.67 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 19 | 0.67 |
| (1,731) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 11 | 0.67 |
| (1,731) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 11 | 0.67 |
| (1,731) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 11 | 0.67 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 10 | 0.67 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 7 | 0.67 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 9 | 0.67 |
| (1,1303) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 10 | 0.67 |
| (1,1303) | 1:B:180:GLY:HA2 | 1:B:181:ILE:HG13 | 10 | 0.67 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 9 | 0.67 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 16 | 0.67 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 6 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 6 | 0.67 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 6 | 0.67 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 9 | 0.67 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 16 | 0.67 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 6 | 0.67 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 6 | 0.67 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 6 | 0.67 |
| (1,970) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 15 | 0.66 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 20 | 0.66 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 20 | 0.66 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 20 | 0.66 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 20 | 0.66 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 20 | 0.66 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 20 | 0.66 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 20 | 0.66 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 20 | 0.66 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 20 | 0.66 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 9 | 0.66 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 9 | 0.66 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 9 | 0.66 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 6 | 0.66 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 9 | 0.66 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 9 | 0.66 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 9 | 0.66 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 9 | 0.66 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 9 | 0.66 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 9 | 0.66 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 9 | 0.66 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 9 | 0.66 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 9 | 0.66 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 3 | 0.66 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 12 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 2 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 2 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 2 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 15 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 15 | 0.66 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 15 | 0.66 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 12 | 0.66 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 2 | 0.66 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 2 | 0.66 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 2 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 15 | 0.66 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 15 | 0.66 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 15 | 0.66 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 20 | 0.65 |
| (1,903) | 1:B:188:THR:HG21 | 1:B:187:LEU:H | 7 | 0.65 |
| (1,903) | 1:B:188:THR:HG22 | 1:B:187:LEU:H | 7 | 0.65 |
| (1,903) | 1:B:188:THR:HG23 | 1:B:187:LEU:H | 7 | 0.65 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 5 | 0.65 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 5 | 0.65 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 5 | 0.65 |
| (1,1691) | 1:B:158:SER:H | 1:B:162:LEU:HG | 10 | 0.65 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 13 | 0.65 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 13 | 0.65 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 13 | 0.65 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 5 | 0.65 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 5 | 0.65 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 5 | 0.65 |
| (1,1376) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 12 | 0.65 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 17 | 0.65 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 17 | 0.65 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 17 | 0.65 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 17 | 0.65 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 17 | 0.65 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 17 | 0.65 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 7 | 0.65 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 9 | 0.65 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 9 | 0.65 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 9 | 0.65 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 11 | 0.65 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 11 | 0.65 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 11 | 0.65 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 7 | 0.65 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 9 | 0.65 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 9 | 0.65 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 9 | 0.65 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 11 | 0.65 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 11 | 0.65 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 11 | 0.65 |
| (1,845) | 1:B:185:ARG:HD2 | 1:B:186:ARG:HB2 | 7 | 0.64 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 19 | 0.64 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 19 | 0.64 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 19 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 7 | 0.64 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 7 | 0.64 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 7 | 0.64 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 7 | 0.64 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 7 | 0.64 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 7 | 0.64 |
| (1,1937) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 6 | 0.64 |
| (1,1937) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 6 | 0.64 |
| (1,1937) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 6 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 4 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 4 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 4 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 8 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 8 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 8 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 9 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 9 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 9 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 14 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 14 | 0.64 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 14 | 0.64 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 6 | 0.64 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 6 | 0.64 |
| (1,1380) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 6 | 0.64 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 6 | 0.64 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 11 | 0.64 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 10 | 0.64 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 10 | 0.64 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 10 | 0.64 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 6 | 0.64 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 11 | 0.64 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 10 | 0.64 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 10 | 0.64 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 10 | 0.64 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 18 | 0.63 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 18 | 0.63 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 18 | 0.63 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 18 | 0.63 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 18 | 0.63 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 18 | 0.63 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 18 | 0.63 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 18 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 18 | 0.63 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 8 | 0.63 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 8 | 0.63 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 8 | 0.63 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 12 | 0.63 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 12 | 0.63 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 12 | 0.63 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 14 | 0.63 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 14 | 0.63 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 14 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 8 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 8 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 8 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 12 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 12 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 12 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 14 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 14 | 0.63 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 14 | 0.63 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 19 | 0.63 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 19 | 0.63 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 19 | 0.63 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 19 | 0.63 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 19 | 0.63 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 19 | 0.63 |
| (1,1953) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 16 | 0.63 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 6 | 0.63 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 6 | 0.63 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 6 | 0.63 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 17 | 0.63 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 17 | 0.63 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 17 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 12 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 12 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 12 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 19 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 19 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 19 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 20 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 20 | 0.63 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 20 | 0.63 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 12 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 12 | 0.63 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 12 | 0.63 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 19 | 0.63 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 19 | 0.63 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 19 | 0.63 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 20 | 0.63 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 20 | 0.63 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 20 | 0.63 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 2 | 0.62 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 11 | 0.62 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 11 | 0.62 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 11 | 0.62 |
| (1,437) | 1:B:188:THR:HG21 | 1:B:187:LEU:HB3 | 7 | 0.62 |
| (1,437) | 1:B:188:THR:HG22 | 1:B:187:LEU:HB3 | 7 | 0.62 |
| (1,437) | 1:B:188:THR:HG23 | 1:B:187:LEU:HB3 | 7 | 0.62 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 17 | 0.62 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 17 | 0.62 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 17 | 0.62 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 20 | 0.62 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 20 | 0.62 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 20 | 0.62 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 10 | 0.62 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 15 | 0.62 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 15 | 0.62 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 15 | 0.62 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 15 | 0.62 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 15 | 0.62 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 15 | 0.62 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 19 | 0.62 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 19 | 0.62 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 19 | 0.62 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 8 | 0.62 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 8 | 0.62 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 20 | 0.61 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 20 | 0.61 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 20 | 0.61 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 20 | 0.61 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 20 | 0.61 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 20 | 0.61 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 6 | 0.61 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 6 | 0.61 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 6 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 9 | 0.61 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 9 | 0.61 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 9 | 0.61 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 3 | 0.61 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 13 | 0.61 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 6 | 0.61 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 6 | 0.61 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 6 | 0.61 |
| (1,1679) | 1:B:157:PHE:H | 1:B:157:PHE:HB2 | 13 | 0.61 |
| (1,1679) | 1:B:157:PHE:H | 1:B:157:PHE:HB2 | 19 | 0.61 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 1 | 0.61 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 1 | 0.61 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 1 | 0.61 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 16 | 0.61 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 16 | 0.61 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 16 | 0.61 |
| (1,1414) | 1:B:157:PHE:H | 1:B:157:PHE:HB2 | 13 | 0.61 |
| (1,1414) | 1:B:157:PHE:H | 1:B:157:PHE:HB2 | 19 | 0.61 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 16 | 0.61 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 14 | 0.61 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 17 | 0.61 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 7 | 0.61 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 7 | 0.61 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 7 | 0.61 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 18 | 0.61 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 18 | 0.61 |
| (1,1212) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 18 | 0.61 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 14 | 0.61 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 17 | 0.61 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 7 | 0.61 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 7 | 0.61 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 7 | 0.61 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD21 | 18 | 0.61 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD22 | 18 | 0.61 |
| (1,1024) | 1:B:170:LEU:HA | 1:B:170:LEU:HD23 | 18 | 0.61 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 7 | 0.6 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 7 | 0.6 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 7 | 0.6 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 17 | 0.6 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 17 | 0.6 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 17 | 0.6 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 17 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 17 | 0.6 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 17 | 0.6 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 3 | 0.59 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 3 | 0.59 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 3 | 0.59 |
| (1,845) | 1:B:185:ARG:HD2 | 1:B:186:ARG:HB2 | 13 | 0.59 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 20 | 0.59 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 15 | 0.59 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 15 | 0.59 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 15 | 0.59 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD11 | 10 | 0.59 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD12 | 10 | 0.59 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HD13 | 10 | 0.59 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG21 | 10 | 0.59 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG22 | 10 | 0.59 |
| (1,1956) | 1:B:183:ILE:HB | 1:B:181:ILE:HG23 | 10 | 0.59 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 10 | 0.59 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 10 | 0.59 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 10 | 0.59 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 5 | 0.58 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 5 | 0.58 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 5 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 1 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 1 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 1 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 7 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 7 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 7 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 12 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 12 | 0.58 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 12 | 0.58 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 19 | 0.58 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 19 | 0.58 |
| (1,1873) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 19 | 0.58 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 2 | 0.57 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 2 | 0.57 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 2 | 0.57 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 2 | 0.57 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 2 | 0.57 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 2 | 0.57 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 1 | 0.57 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 1 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 1 | 0.57 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 16 | 0.57 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 16 | 0.57 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 16 | 0.57 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 19 | 0.57 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 9 | 0.57 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 9 | 0.57 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 9 | 0.57 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 1 | 0.57 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 1 | 0.57 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 1 | 0.57 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 16 | 0.57 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 16 | 0.57 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 16 | 0.57 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 19 | 0.57 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 20 | 0.57 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 20 | 0.57 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 20 | 0.57 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 10 | 0.57 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 18 | 0.56 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 17 | 0.56 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 17 | 0.56 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 17 | 0.56 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 17 | 0.56 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 17 | 0.56 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 17 | 0.56 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 17 | 0.56 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 17 | 0.56 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 17 | 0.56 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 20 | 0.56 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 20 | 0.56 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 20 | 0.56 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 20 | 0.56 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 20 | 0.56 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 20 | 0.56 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 2 | 0.56 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 6 | 0.56 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 6 | 0.56 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 6 | 0.56 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 6 | 0.56 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 6 | 0.56 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 6 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 7 | 0.56 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 7 | 0.56 |
| (1,1575) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 7 | 0.56 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 3 | 0.55 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 3 | 0.55 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 3 | 0.55 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 3 | 0.55 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 3 | 0.55 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 3 | 0.55 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 3 | 0.55 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 3 | 0.55 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 3 | 0.55 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 1 | 0.55 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 4 | 0.55 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 11 | 0.55 |
| (1,1425) | 1:B:158:SER:H | 1:B:162:LEU:HG | 10 | 0.55 |
| (1,566) | 1:B:163:LYS:HD2 | 1:B:160:GLU:HA | 16 | 0.54 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 2 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 14 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 14 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 14 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 14 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 14 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 14 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 20 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 20 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 20 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 20 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 20 | 0.54 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 20 | 0.54 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 8 | 0.53 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 8 | 0.53 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 8 | 0.53 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 8 | 0.53 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 8 | 0.53 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 8 | 0.53 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 8 | 0.53 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 8 | 0.53 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 8 | 0.53 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 9 | 0.53 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 9 | 0.53 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 9 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 9 | 0.53 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 9 | 0.53 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 9 | 0.53 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 9 | 0.53 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 9 | 0.53 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 9 | 0.53 |
| (1,772) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 7 | 0.53 |
| (1,772) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 7 | 0.53 |
| (1,772) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 7 | 0.53 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 4 | 0.53 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 4 | 0.53 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 4 | 0.53 |
| (1,1975) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA2 | 7 | 0.53 |
| (1,1975) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA2 | 7 | 0.53 |
| (1,1975) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA2 | 7 | 0.53 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 4 | 0.53 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 4 | 0.53 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 4 | 0.53 |
| (1,846) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 5 | 0.52 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 7 | 0.52 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 7 | 0.52 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 7 | 0.52 |
| (1,572) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 16 | 0.52 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 7 | 0.52 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 7 | 0.52 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 7 | 0.52 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 8 | 0.52 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 18 | 0.52 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 4 | 0.52 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 4 | 0.52 |
| (1,1980) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 4 | 0.52 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 11 | 0.52 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 11 | 0.52 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 11 | 0.52 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 15 | 0.52 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 15 | 0.52 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 15 | 0.52 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG21 | 4 | 0.52 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG22 | 4 | 0.52 |
| (1,1948) | 1:B:179:LEU:HG | 1:B:177:ILE:HG23 | 4 | 0.52 |
| (1,1699) | 1:B:160:GLU:H | 1:B:158:SER:HB3 | 4 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 3 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 3 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 3 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 3 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 3 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 3 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 8 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 8 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 8 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 8 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 8 | 0.52 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 8 | 0.52 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 3 | 0.52 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 3 | 0.52 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 6 | 0.51 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 6 | 0.51 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 6 | 0.51 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 13 | 0.51 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 13 | 0.51 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 13 | 0.51 |
| (1,572) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 3 | 0.51 |
| (1,572) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 5 | 0.51 |
| (1,572) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 8 | 0.51 |
| (1,572) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 12 | 0.51 |
| (1,572) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 19 | 0.51 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 13 | 0.51 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 13 | 0.51 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 13 | 0.51 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 5 | 0.51 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 12 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 2 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 2 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 2 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 2 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 2 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 2 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 4 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 4 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 4 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 4 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 4 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 4 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 18 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 18 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 18 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 18 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 18 | 0.51 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 18 | 0.51 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 18 | 0.51 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 18 | 0.51 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 19 | 0.5 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 14 | 0.5 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 14 | 0.5 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 14 | 0.5 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 14 | 0.5 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 14 | 0.5 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 14 | 0.5 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 17 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 11 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 11 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 11 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 11 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 11 | 0.5 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 11 | 0.5 |
| (1,903) | 1:B:188:THR:HG21 | 1:B:187:LEU:H | 8 | 0.49 |
| (1,903) | 1:B:188:THR:HG22 | 1:B:187:LEU:H | 8 | 0.49 |
| (1,903) | 1:B:188:THR:HG23 | 1:B:187:LEU:H | 8 | 0.49 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 18 | 0.49 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 18 | 0.49 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 18 | 0.49 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 19 | 0.49 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 19 | 0.49 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 19 | 0.49 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 18 | 0.49 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 18 | 0.49 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 18 | 0.49 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 19 | 0.49 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 19 | 0.49 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 19 | 0.49 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 12 | 0.49 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 12 | 0.49 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 12 | 0.49 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 12 | 0.49 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 12 | 0.49 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 12 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 12 | 0.49 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 12 | 0.49 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 12 | 0.49 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 19 | 0.49 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 19 | 0.49 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 19 | 0.49 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 19 | 0.49 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 19 | 0.49 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 19 | 0.49 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 2 | 0.49 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 5 | 0.49 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 2 | 0.49 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 5 | 0.49 |
| (1,953) | 1:B:158:SER:HB2 | 1:B:155:GLY:H | 5 | 0.48 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 3 | 0.48 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 3 | 0.48 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 3 | 0.48 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 9 | 0.48 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 9 | 0.48 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 9 | 0.48 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 11 | 0.48 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 11 | 0.48 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 11 | 0.48 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 2 | 0.48 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 2 | 0.48 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 2 | 0.48 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 3 | 0.48 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 3 | 0.48 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 3 | 0.48 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 9 | 0.48 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 9 | 0.48 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 9 | 0.48 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 11 | 0.48 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 11 | 0.48 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 11 | 0.48 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 18 | 0.48 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 5 | 0.48 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 5 | 0.48 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 5 | 0.48 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 5 | 0.48 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 5 | 0.48 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,846) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 18 | 0.47 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 6 | 0.47 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 6 | 0.47 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 6 | 0.47 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 10 | 0.47 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 10 | 0.47 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 10 | 0.47 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 15 | 0.47 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 15 | 0.47 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 15 | 0.47 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 16 | 0.47 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 16 | 0.47 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 16 | 0.47 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 17 | 0.47 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 17 | 0.47 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 17 | 0.47 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 6 | 0.47 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 6 | 0.47 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 6 | 0.47 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 10 | 0.47 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 10 | 0.47 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 10 | 0.47 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 15 | 0.47 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 15 | 0.47 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 15 | 0.47 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 16 | 0.47 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 16 | 0.47 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 16 | 0.47 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 17 | 0.47 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 17 | 0.47 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 17 | 0.47 |
| (1,261) | 1:B:170:LEU:HD21 | 1:B:166:LEU:HB2 | 11 | 0.47 |
| (1,261) | 1:B:170:LEU:HD22 | 1:B:166:LEU:HB2 | 11 | 0.47 |
| (1,261) | 1:B:170:LEU:HD23 | 1:B:166:LEU:HB2 | 11 | 0.47 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 7 | 0.47 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 9 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 1 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 1 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 1 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 2 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 2 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 2 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 3 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 3 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 3 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 5 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 5 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 5 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 6 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 6 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 6 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 16 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 16 | 0.47 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 16 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 9 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 9 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 9 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 9 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 9 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 9 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 13 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 13 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 13 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 13 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 13 | 0.47 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 13 | 0.47 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 9 | 0.47 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 4 | 0.46 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 16 | 0.46 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 16 | 0.46 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 16 | 0.46 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 16 | 0.46 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 16 | 0.46 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 16 | 0.46 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 16 | 0.46 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 16 | 0.46 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 16 | 0.46 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 2 | 0.46 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 2 | 0.46 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 2 | 0.46 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 4 | 0.46 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 4 | 0.46 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 4 | 0.46 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 2 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 2 | 0.46 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 2 | 0.46 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 4 | 0.46 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 4 | 0.46 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 4 | 0.46 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 20 | 0.46 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 20 | 0.46 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 20 | 0.46 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 9 | 0.46 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 9 | 0.46 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 9 | 0.46 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 14 | 0.46 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 1 | 0.46 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 1 | 0.46 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 1 | 0.46 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 1 | 0.46 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 1 | 0.46 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 1 | 0.46 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 15 | 0.46 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 15 | 0.46 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 6 | 0.45 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 6 | 0.45 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 6 | 0.45 |
| (2,30) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 11 | 0.45 |
| (2,26) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 11 | 0.45 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 6 | 0.45 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 6 | 0.45 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 6 | 0.45 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 1 | 0.45 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 1 | 0.45 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 1 | 0.45 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 5 | 0.45 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 5 | 0.45 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 5 | 0.45 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 8 | 0.45 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 8 | 0.45 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 8 | 0.45 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 16 | 0.45 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 16 | 0.45 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 16 | 0.45 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 1 | 0.45 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 1 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 1 | 0.45 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 5 | 0.45 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 5 | 0.45 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 5 | 0.45 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 8 | 0.45 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 8 | 0.45 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 8 | 0.45 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 8 | 0.45 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 8 | 0.45 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 8 | 0.45 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 10 | 0.45 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 10 | 0.45 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 10 | 0.45 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 5 | 0.45 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 5 | 0.45 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 5 | 0.45 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 2 | 0.45 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 2 | 0.45 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 2 | 0.45 |
| (1,1699) | 1:B:160:GLU:H | 1:B:158:SER:HB3 | 3 | 0.45 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 13 | 0.45 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 13 | 0.45 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 12 | 0.44 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 12 | 0.44 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 12 | 0.44 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 18 | 0.44 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 18 | 0.44 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 18 | 0.44 |
| (1,376) | 1:B:185:ARG:HD2 | 1:B:186:ARG:HB2 | 7 | 0.44 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 12 | 0.44 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 12 | 0.44 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 12 | 0.44 |
| (1,1970) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 6 | 0.44 |
| (1,1970) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 6 | 0.44 |
| (1,1970) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 6 | 0.44 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 10 | 0.44 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 10 | 0.44 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 10 | 0.44 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 16 | 0.44 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 17 | 0.44 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 17 | 0.44 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 17 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 17 | 0.44 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 17 | 0.44 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 17 | 0.44 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 2 | 0.44 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 18 | 0.43 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 18 | 0.43 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 18 | 0.43 |
| (1,970) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 7 | 0.43 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 2 | 0.43 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 2 | 0.43 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 2 | 0.43 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 14 | 0.43 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 14 | 0.43 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 14 | 0.43 |
| (1,1985) | 1:B:181:ILE:HA | 1:B:184:GLY:HA2 | 16 | 0.43 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 18 | 0.43 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 18 | 0.43 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 18 | 0.43 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 3 | 0.43 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 3 | 0.43 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 3 | 0.43 |
| (1,1691) | 1:B:158:SER:H | 1:B:162:LEU:HG | 6 | 0.43 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 13 | 0.43 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 13 | 0.43 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 13 | 0.43 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 13 | 0.43 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 13 | 0.43 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 13 | 0.43 |
| (1,1282) | 1:B:186:ARG:HA | 1:B:186:ARG:HD3 | 13 | 0.43 |
| (1,1159) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 11 | 0.43 |
| (1,766) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 20 | 0.42 |
| (1,766) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 20 | 0.42 |
| (1,766) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 20 | 0.42 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 3 | 0.42 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 3 | 0.42 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 3 | 0.42 |
| (1,296) | 1:B:177:ILE:HD11 | 1:B:176:ALA:HA | 20 | 0.42 |
| (1,296) | 1:B:177:ILE:HD12 | 1:B:176:ALA:HA | 20 | 0.42 |
| (1,296) | 1:B:177:ILE:HD13 | 1:B:176:ALA:HA | 20 | 0.42 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 7 | 0.42 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 7 | 0.42 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 7 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 15 | 0.42 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 15 | 0.42 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 15 | 0.42 |
| (1,1699) | 1:B:160:GLU:H | 1:B:158:SER:HB3 | 7 | 0.42 |
| (1,1699) | 1:B:160:GLU:H | 1:B:158:SER:HB3 | 18 | 0.42 |
| (1,1699) | 1:B:160:GLU:H | 1:B:158:SER:HB3 | 20 | 0.42 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 16 | 0.42 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 16 | 0.42 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 16 | 0.42 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 16 | 0.42 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 16 | 0.42 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 16 | 0.42 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 20 | 0.42 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 10 | 0.42 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 10 | 0.42 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 10 | 0.42 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 10 | 0.42 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 10 | 0.42 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 10 | 0.42 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 20 | 0.41 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 15 | 0.41 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 15 | 0.41 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 15 | 0.41 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 18 | 0.41 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 18 | 0.41 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 18 | 0.41 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 3 | 0.41 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 7 | 0.41 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 7 | 0.41 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 7 | 0.41 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD11 | 7 | 0.41 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD12 | 7 | 0.41 |
| (1,1604) | 1:B:184:GLY:H | 1:B:181:ILE:HD13 | 7 | 0.41 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 1 | 0.41 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 5 | 0.4 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 5 | 0.4 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 5 | 0.4 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 11 | 0.4 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 11 | 0.4 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 11 | 0.4 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 6 | 0.4 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 5 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 15 | 0.4 |
| (1,1282) | 1:B:186:ARG:HA | 1:B:186:ARG:HD3 | 11 | 0.4 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 7 | 0.39 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 7 | 0.39 |
| (2,5) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 7 | 0.39 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 7 | 0.39 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 7 | 0.39 |
| (2,5) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 7 | 0.39 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 7 | 0.39 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 7 | 0.39 |
| (2,5) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 7 | 0.39 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 8 | 0.39 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 8 | 0.39 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 8 | 0.39 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 2 | 0.39 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 2 | 0.39 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 2 | 0.39 |
| (1,376) | 1:B:185:ARG:HD2 | 1:B:186:ARG:HB2 | 13 | 0.39 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 17 | 0.39 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 17 | 0.39 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 17 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 1 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 1 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 1 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 1 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 1 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 1 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 2 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 2 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 2 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 2 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 2 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 2 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 3 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 3 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 3 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 3 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 3 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 3 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 4 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 4 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 4 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 4 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 4 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 4 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 5 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 5 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 5 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 5 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 5 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 5 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 6 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 6 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 6 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 6 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 6 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 6 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 7 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 7 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 7 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 7 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 7 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 7 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 8 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 8 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 8 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 8 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 8 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 8 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 9 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 9 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 9 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 9 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 9 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 9 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 10 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 10 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 10 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 10 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 10 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 10 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 11 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 11 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 11 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 11 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 11 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 11 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 12 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 12 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 12 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 12 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 12 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 12 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 13 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 13 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 13 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 13 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 13 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 13 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 14 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 14 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 14 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 14 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 14 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 14 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 15 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 15 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 15 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 15 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 15 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 15 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 16 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 16 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 16 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 16 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 16 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 16 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 17 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 17 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 17 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 17 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 17 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 17 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 18 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 18 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 18 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 18 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 18 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 18 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 19 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 19 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 19 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 19 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 19 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 19 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB2 | 20 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB1 | 1:B:176:ALA:HB3 | 20 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB1 | 20 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB2 | 1:B:176:ALA:HB3 | 20 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB1 | 20 | 0.39 |
| (1,1938) | 1:B:176:ALA:HB3 | 1:B:176:ALA:HB2 | 20 | 0.39 |
| (1,1691) | 1:B:158:SER:H | 1:B:162:LEU:HG | 17 | 0.39 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 4 | 0.39 |
| (1,970) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 13 | 0.38 |
| (1,846) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 10 | 0.38 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 8 | 0.38 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 8 | 0.38 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 8 | 0.38 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 14 | 0.38 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 14 | 0.38 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 14 | 0.38 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 9 | 0.38 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 9 | 0.38 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 9 | 0.38 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 9 | 0.38 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 9 | 0.38 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 9 | 0.38 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 12 | 0.38 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 12 | 0.38 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 12 | 0.38 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 13 | 0.38 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 10 | 0.38 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 10 | 0.38 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 8 | 0.37 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 20 | 0.37 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 19 | 0.36 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 19 | 0.36 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 19 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1670) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 17 | 0.36 |
| (1,1670) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 19 | 0.36 |
| (1,1670) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 20 | 0.36 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 16 | 0.36 |
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 4 | 0.36 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 4 | 0.36 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 1 | 0.35 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 1 | 0.35 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 1 | 0.35 |
| (1,953) | 1:B:158:SER:HB2 | 1:B:155:GLY:H | 19 | 0.35 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 4 | 0.35 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 4 | 0.35 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 4 | 0.35 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 13 | 0.35 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 13 | 0.35 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 13 | 0.35 |
| (1,1670) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 13 | 0.35 |
| (1,1670) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 15 | 0.35 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 4 | 0.35 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 14 | 0.34 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 14 | 0.34 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 14 | 0.34 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 18 | 0.34 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 18 | 0.34 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 18 | 0.34 |
| (1,1977) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 13 | 0.34 |
| (1,1977) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 13 | 0.34 |
| (1,1977) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 13 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 4 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 4 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 4 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 8 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 8 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 8 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 9 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 9 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 9 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 14 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 14 | 0.34 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 14 | 0.34 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 8 | 0.34 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 17 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1244) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 19 | 0.34 |
| (1,108) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HG2 | 2 | 0.34 |
| (1,108) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HG2 | 6 | 0.34 |
| (1,108) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HG2 | 18 | 0.34 |
| (1,1056) | 1:B:176:ALA:HA | 1:B:179:LEU:HB3 | 19 | 0.34 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 10 | 0.33 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 10 | 0.33 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 10 | 0.33 |
| (1,957) | 1:B:158:SER:HB3 | 1:B:159:ALA:H | 16 | 0.33 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 1 | 0.33 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 1 | 0.33 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 1 | 0.33 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 6 | 0.33 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 6 | 0.33 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 6 | 0.33 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 4 | 0.33 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 4 | 0.33 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 4 | 0.33 |
| (1,398) | 1:B:186:ARG:HD3 | 1:B:182:TYR:HE1 | 20 | 0.33 |
| (1,398) | 1:B:186:ARG:HD3 | 1:B:182:TYR:HE2 | 20 | 0.33 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 11 | 0.33 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 11 | 0.33 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 11 | 0.33 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 11 | 0.33 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 11 | 0.33 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 11 | 0.33 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 6 | 0.33 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 6 | 0.33 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 6 | 0.33 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 17 | 0.33 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 17 | 0.33 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 17 | 0.33 |
| (1,1428) | 1:B:159:ALA:H | 1:B:158:SER:HB3 | 16 | 0.33 |
| (1,1425) | 1:B:158:SER:H | 1:B:162:LEU:HG | 6 | 0.33 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 19 | 0.33 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 19 | 0.33 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 19 | 0.33 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 19 | 0.33 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 19 | 0.33 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 19 | 0.33 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 10 | 0.32 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 10 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 10 | 0.32 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 19 | 0.32 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 19 | 0.32 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 19 | 0.32 |
| (1,1888) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 13 | 0.32 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 19 | 0.32 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 19 | 0.32 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 19 | 0.32 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 1 | 0.32 |
| (1,104) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 16 | 0.32 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 17 | 0.31 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 17 | 0.31 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 17 | 0.31 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 17 | 0.31 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 17 | 0.31 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 17 | 0.31 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD11 | 5 | 0.31 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD12 | 5 | 0.31 |
| (1,905) | 1:B:188:THR:HG21 | 1:B:187:LEU:HD13 | 5 | 0.31 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD11 | 5 | 0.31 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD12 | 5 | 0.31 |
| (1,905) | 1:B:188:THR:HG22 | 1:B:187:LEU:HD13 | 5 | 0.31 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD11 | 5 | 0.31 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD12 | 5 | 0.31 |
| (1,905) | 1:B:188:THR:HG23 | 1:B:187:LEU:HD13 | 5 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 2 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 2 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 2 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 2 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 2 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 2 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 3 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 3 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 3 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 3 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 3 | 0.31 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 3 | 0.31 |
| (1,1888) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 11 | 0.31 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 1 | 0.31 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 1 | 0.31 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 1 | 0.31 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 16 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 16 | 0.31 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 16 | 0.31 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 3 | 0.31 |
| (1,105) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HB3 | 17 | 0.31 |
| (1,104) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 3 | 0.31 |
| (1,104) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 5 | 0.31 |
| (1,104) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 8 | 0.31 |
| (1,104) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 12 | 0.31 |
| (1,104) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HG2 | 19 | 0.31 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 1 | 0.3 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 3 | 0.3 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 12 | 0.3 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 12 | 0.3 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 12 | 0.3 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 20 | 0.3 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 20 | 0.3 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 20 | 0.3 |
| (1,398) | 1:B:186:ARG:HD3 | 1:B:182:TYR:HE1 | 6 | 0.3 |
| (1,398) | 1:B:186:ARG:HD3 | 1:B:182:TYR:HE2 | 6 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 10 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 10 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 10 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 10 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 10 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 10 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 12 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 12 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 12 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 12 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 12 | 0.3 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 12 | 0.3 |
| (1,1888) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 2 | 0.3 |
| (1,1888) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 7 | 0.3 |
| (1,1848) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 20 | 0.3 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 20 | 0.3 |
| (1,1579) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 20 | 0.3 |
| (1,1415) | 1:B:157:PHE:H | 1:B:157:PHE:HB3 | 9 | 0.3 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 14 | 0.3 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 14 | 0.3 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 14 | 0.3 |
| (1,811) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 15 | 0.29 |
| (1,811) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 15 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,811) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 15 | 0.29 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 11 | 0.29 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 11 | 0.29 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 11 | 0.29 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 13 | 0.29 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 13 | 0.29 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 13 | 0.29 |
| (1,1950) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 15 | 0.29 |
| (1,1950) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 15 | 0.29 |
| (1,1950) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 15 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 5 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 5 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 5 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 5 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 5 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 5 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 6 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 6 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 6 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 6 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 6 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 6 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 20 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 20 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 20 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 20 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 20 | 0.29 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 20 | 0.29 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 15 | 0.29 |
| (1,1730) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 3 | 0.29 |
| (1,1730) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 8 | 0.29 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 15 | 0.29 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 16 | 0.29 |
| (1,148) | 1:B:166:LEU:HB3 | 1:B:167:PRO:HD2 | 6 | 0.29 |
| (1,1462) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 3 | 0.29 |
| (1,1462) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 8 | 0.29 |
| (1,1425) | 1:B:158:SER:H | 1:B:162:LEU:HG | 17 | 0.29 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 18 | 0.28 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 18 | 0.28 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 18 | 0.28 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 2 | 0.28 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 2 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 2 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 1 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 1 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 1 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 1 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 1 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 1 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 8 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 8 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 8 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 8 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 8 | 0.28 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 8 | 0.28 |
| (1,1730) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 12 | 0.28 |
| (1,1730) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 19 | 0.28 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 12 | 0.28 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 14 | 0.28 |
| (1,1462) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 12 | 0.28 |
| (1,1462) | 1:B:163:LYS:H | 1:B:163:LYS:HB2 | 19 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 6 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 6 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 6 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 6 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 6 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 6 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 15 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 15 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 15 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 15 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 15 | 0.28 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 15 | 0.28 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 7 | 0.27 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 7 | 0.27 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 7 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 16 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 16 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 16 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 16 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 16 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 16 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 18 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 18 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 18 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 18 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 18 | 0.27 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 18 | 0.27 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 20 | 0.27 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 20 | 0.27 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 20 | 0.27 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 13 | 0.27 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 6 | 0.27 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 8 | 0.27 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 2 | 0.26 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 2 | 0.26 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 2 | 0.26 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 16 | 0.26 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 16 | 0.26 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 16 | 0.26 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 1 | 0.26 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 1 | 0.26 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 1 | 0.26 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 20 | 0.26 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 20 | 0.26 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 20 | 0.26 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 14 | 0.26 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG21 | 7 | 0.26 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG22 | 7 | 0.26 |
| (1,1844) | 1:B:180:GLY:H | 1:B:177:ILE:HG23 | 7 | 0.26 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 14 | 0.26 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 9 | 0.26 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 17 | 0.26 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 9 | 0.26 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 9 | 0.26 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 9 | 0.26 |
| (2,30) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 16 | 0.25 |
| (2,26) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 16 | 0.25 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 7 | 0.25 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 7 | 0.25 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 7 | 0.25 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 2 | 0.25 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 2 | 0.25 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 2 | 0.25 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 10 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 10 | 0.25 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 2 | 0.25 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 2 | 0.25 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 2 | 0.25 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 15 | 0.25 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 15 | 0.25 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 15 | 0.25 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 15 | 0.25 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 15 | 0.25 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 15 | 0.25 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 19 | 0.25 |
| (1,148) | 1:B:166:LEU:HB3 | 1:B:167:PRO:HD2 | 3 | 0.25 |
| (1,95) | 1:B:163:LYS:HD2 | 1:B:160:GLU:HA | 16 | 0.24 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 10 | 0.24 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 10 | 0.24 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 10 | 0.24 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 10 | 0.24 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 10 | 0.24 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 10 | 0.24 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 3 | 0.24 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 7 | 0.24 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 3 | 0.24 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 7 | 0.24 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD21 | 17 | 0.23 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD22 | 17 | 0.23 |
| (1,997) | 1:B:165:PHE:HA | 1:B:169:LEU:HD23 | 17 | 0.23 |
| (1,972) | 1:B:160:GLU:HA | 1:B:163:LYS:HG2 | 11 | 0.23 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 3 | 0.23 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 3 | 0.23 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 3 | 0.23 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 3 | 0.23 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 3 | 0.23 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 7 | 0.23 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 7 | 0.23 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 7 | 0.23 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 7 | 0.23 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 7 | 0.23 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 7 | 0.23 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 8 | 0.23 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 8 | 0.23 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 8 | 0.23 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 8 | 0.23 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 8 | 0.23 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 8 | 0.23 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 1 | 0.23 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 1 | 0.23 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 1 | 0.23 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 3 | 0.23 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 3 | 0.23 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 3 | 0.23 |
| (1,1094) | 1:B:186:ARG:HA | 1:B:186:ARG:HD3 | 13 | 0.23 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 1 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 2 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 3 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 4 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 5 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 6 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 7 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 8 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 9 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 10 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 11 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 12 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 13 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 14 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 15 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 16 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 17 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 18 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 19 | 0.22 |
| (1,783) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 20 | 0.22 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 15 | 0.22 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 15 | 0.22 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 15 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 17 | 0.22 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 17 | 0.22 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 17 | 0.22 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 20 | 0.22 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 20 | 0.22 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 20 | 0.22 |
| (1,377) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 5 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 1 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 2 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 3 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 4 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 5 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 6 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 7 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 8 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 9 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 10 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 11 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 12 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 13 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 14 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 15 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 16 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 17 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 18 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 19 | 0.22 |
| (1,314) | 1:B:179:LEU:HB3 | 1:B:179:LEU:HG | 20 | 0.22 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 20 | 0.22 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 20 | 0.22 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 20 | 0.22 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 15 | 0.22 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 15 | 0.22 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 15 | 0.22 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 17 | 0.22 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 17 | 0.22 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 17 | 0.22 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 17 | 0.22 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 17 | 0.22 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 17 | 0.22 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 1 | 0.22 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 2 | 0.22 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 10 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 1 | 0.22 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 1 | 0.22 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 2 | 0.22 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 10 | 0.22 |
| (1,1619) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 13 | 0.22 |
| (1,1614) | 1:B:185:ARG:H | 1:B:185:ARG:HG2 | 11 | 0.22 |
| (1,148) | 1:B:166:LEU:HB3 | 1:B:167:PRO:HD2 | 7 | 0.22 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 9 | 0.22 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 2 | 0.22 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 2 | 0.22 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 2 | 0.22 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 18 | 0.22 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 18 | 0.22 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 18 | 0.22 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 11 | 0.21 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 11 | 0.21 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 11 | 0.21 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 11 | 0.21 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 11 | 0.21 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 11 | 0.21 |
| (1,83) | 1:B:162:LEU:HD21 | 1:B:166:LEU:HG | 10 | 0.21 |
| (1,83) | 1:B:162:LEU:HD22 | 1:B:166:LEU:HG | 10 | 0.21 |
| (1,83) | 1:B:162:LEU:HD23 | 1:B:166:LEU:HG | 10 | 0.21 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 18 | 0.21 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 18 | 0.21 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 18 | 0.21 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 4 | 0.21 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 4 | 0.21 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 4 | 0.21 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 12 | 0.21 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 12 | 0.21 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 12 | 0.21 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 18 | 0.21 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 18 | 0.21 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 18 | 0.21 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 14 | 0.21 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 14 | 0.21 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 14 | 0.21 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 14 | 0.21 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 14 | 0.21 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 14 | 0.21 |
| (1,1699) | 1:B:160:GLU:H | 1:B:158:SER:HB3 | 12 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1619) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 11 | 0.21 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 6 | 0.21 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 7 | 0.21 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 4 | 0.21 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 4 | 0.21 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 4 | 0.21 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 20 | 0.21 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 20 | 0.21 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 20 | 0.21 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 8 | 0.2 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 8 | 0.2 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 8 | 0.2 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 5 | 0.2 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 5 | 0.2 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 5 | 0.2 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 11 | 0.2 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 11 | 0.2 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 11 | 0.2 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 5 | 0.2 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 5 | 0.2 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 5 | 0.2 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 11 | 0.2 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 11 | 0.2 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 11 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 4 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 4 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 4 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 4 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 4 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 4 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 19 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 19 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 19 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 19 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 19 | 0.2 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 19 | 0.2 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 5 | 0.2 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 20 | 0.2 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 5 | 0.2 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 20 | 0.2 |
| (1,1619) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 2 | 0.2 |
| (1,1619) | 1:B:186:ARG:H | 1:B:186:ARG:HB2 | 7 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1419) | 1:B:158:SER:H | 1:B:158:SER:HB2 | 4 | 0.2 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 11 | 0.2 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 16 | 0.2 |
| (1,1094) | 1:B:186:ARG:HA | 1:B:186:ARG:HD3 | 11 | 0.2 |
| (1,105) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HB3 | 7 | 0.2 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 1 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 2 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 4 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 5 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 6 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 7 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 8 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 9 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 10 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 12 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 13 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 14 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 18 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 19 | 0.19 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 20 | 0.19 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 3 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 1 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 2 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 4 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 5 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 6 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 7 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 8 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 9 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 10 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 12 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 13 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 14 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 18 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 19 | 0.19 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 20 | 0.19 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 14 | 0.19 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 14 | 0.19 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 14 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 1 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 4 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 5 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 7 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 8 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 9 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 10 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 11 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 12 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 14 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 15 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 16 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 17 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 18 | 0.19 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 19 | 0.19 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 11 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 1 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 4 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 5 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 7 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 8 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 9 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 10 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 11 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 12 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 14 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 15 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 16 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 17 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 18 | 0.19 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 19 | 0.19 |
| (1,148) | 1:B:166:LEU:HB3 | 1:B:167:PRO:HD2 | 10 | 0.19 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 1 | 0.19 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 4 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 12 | 0.19 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 14 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD11 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD12 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD13 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD11 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD12 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD13 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD11 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD12 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD13 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD11 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD12 | 16 | 0.19 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD13 | 16 | 0.19 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 3 | 0.19 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 3 | 0.19 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 3 | 0.19 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 3 | 0.19 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 3 | 0.19 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 3 | 0.19 |
| (1,926) | 1:B:163:LYS:HE3 | 1:B:159:ALA:HB1 | 5 | 0.18 |
| (1,926) | 1:B:163:LYS:HE3 | 1:B:159:ALA:HB2 | 5 | 0.18 |
| (1,926) | 1:B:163:LYS:HE3 | 1:B:159:ALA:HB3 | 5 | 0.18 |
| (1,858) | 1:B:185:ARG:HG2 | 1:B:186:ARG:HG3 | 16 | 0.18 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 12 | 0.18 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 12 | 0.18 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 12 | 0.18 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 1 | 0.18 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 1 | 0.18 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 1 | 0.18 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 7 | 0.18 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 7 | 0.18 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 7 | 0.18 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 12 | 0.18 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 12 | 0.18 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 12 | 0.18 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 3 | 0.18 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 11 | 0.18 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 15 | 0.18 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 16 | 0.18 |
| (1,695) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 17 | 0.18 |
| (1,390) | 1:B:185:ARG:HG2 | 1:B:186:ARG:HG3 | 16 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 14 | 0.18 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 16 | 0.18 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 17 | 0.18 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 3 | 0.18 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 11 | 0.18 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 15 | 0.18 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 16 | 0.18 |
| (1,225) | 1:B:171:LEU:HB3 | 1:B:171:LEU:H | 17 | 0.18 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 12 | 0.18 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 12 | 0.18 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 12 | 0.18 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HB2 | 13 | 0.18 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HB2 | 13 | 0.18 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HB2 | 13 | 0.18 |
| (1,1945) | 1:B:177:ILE:HG21 | 1:B:183:ILE:HB | 13 | 0.18 |
| (1,1945) | 1:B:177:ILE:HG22 | 1:B:183:ILE:HB | 13 | 0.18 |
| (1,1945) | 1:B:177:ILE:HG23 | 1:B:183:ILE:HB | 13 | 0.18 |
| (1,1848) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 17 | 0.18 |
| (1,1848) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 18 | 0.18 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 2 | 0.18 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 3 | 0.18 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 6 | 0.18 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 13 | 0.18 |
| (1,1836) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 20 | 0.18 |
| (1,1664) | 1:B:156:ILE:H | 1:B:155:GLY:HA2 | 5 | 0.18 |
| (1,1579) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 17 | 0.18 |
| (1,1579) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 18 | 0.18 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 2 | 0.18 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 3 | 0.18 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 6 | 0.18 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 13 | 0.18 |
| (1,1567) | 1:B:179:LEU:H | 1:B:179:LEU:HB3 | 20 | 0.18 |
| (1,148) | 1:B:166:LEU:HB3 | 1:B:167:PRO:HD2 | 5 | 0.18 |
| (1,1419) | 1:B:158:SER:H | 1:B:158:SER:HB2 | 20 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD11 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD12 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD13 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD11 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD12 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD13 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD11 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD12 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD13 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD11 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD12 | 9 | 0.18 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD13 | 9 | 0.18 |
| (1,1142) | 1:B:158:SER:HB2 | 1:B:155:GLY:H | 5 | 0.18 |
| (1,105) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HB3 | 13 | 0.18 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 6 | 0.17 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 6 | 0.17 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 6 | 0.17 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 9 | 0.17 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 19 | 0.17 |
| (1,377) | 1:B:185:ARG:HD3 | 1:B:186:ARG:HB2 | 18 | 0.17 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 12 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 2 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 2 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 2 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 6 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 6 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 6 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 11 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 11 | 0.17 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 11 | 0.17 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 19 | 0.17 |
| (1,1848) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 2 | 0.17 |
| (1,1848) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 12 | 0.17 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 17 | 0.17 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 19 | 0.17 |
| (1,1579) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 2 | 0.17 |
| (1,1579) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 12 | 0.17 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 18 | 0.17 |
| (1,1419) | 1:B:158:SER:H | 1:B:158:SER:HB2 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1419) | 1:B:158:SER:H | 1:B:158:SER:HB2 | 18 | 0.17 |
| (1,1400) | 1:B:156:ILE:H | 1:B:155:GLY:HA3 | 2 | 0.17 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 16 | 0.17 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 16 | 0.17 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 16 | 0.17 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 16 | 0.17 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 16 | 0.17 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 16 | 0.17 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 7 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD11 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD12 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD13 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD11 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD12 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD13 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD11 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD12 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD13 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD11 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD12 | 11 | 0.17 |
| (1,1333) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD13 | 11 | 0.17 |
| (1,1307) | 1:B:165:PHE:HA | 1:B:168:SER:HB2 | 8 | 0.17 |
| (1,972) | 1:B:160:GLU:HA | 1:B:163:LYS:HG2 | 1 | 0.16 |
| (1,83) | 1:B:162:LEU:HD21 | 1:B:166:LEU:HG | 15 | 0.16 |
| (1,83) | 1:B:162:LEU:HD22 | 1:B:166:LEU:HG | 15 | 0.16 |
| (1,83) | 1:B:162:LEU:HD23 | 1:B:166:LEU:HG | 15 | 0.16 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 1 | 0.16 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 3 | 0.16 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 6 | 0.16 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 8 | 0.16 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 11 | 0.16 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 12 | 0.16 |
| (1,386) | 1:B:185:ARG:HG3 | 1:B:185:ARG:HB2 | 20 | 0.16 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 2 | 0.16 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 14 | 0.16 |
| (1,1405) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 17 | 0.16 |
| (1,1405) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 19 | 0.16 |
| (1,1405) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 20 | 0.16 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 5 | 0.16 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 18 | 0.16 |
| (1,971) | 1:B:160:GLU:HA | 1:B:163:LYS:HD3 | 15 | 0.15 |
| (1,96) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HB2 | 4 | 0.15 |
| (1,96) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HB2 | 18 | 0.15 |
| (1,902) | 1:B:188:THR:HG21 | 1:B:185:ARG:HA | 1 | 0.15 |
| (1,902) | 1:B:188:THR:HG22 | 1:B:185:ARG:HA | 1 | 0.15 |
| (1,902) | 1:B:188:THR:HG23 | 1:B:185:ARG:HA | 1 | 0.15 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 13 | 0.15 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 13 | 0.15 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 13 | 0.15 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 4 | 0.15 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 4 | 0.15 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 4 | 0.15 |
| (1,369) | 1:B:185:ARG:HD3 | 1:B:182:TYR:HD1 | 15 | 0.15 |
| (1,369) | 1:B:185:ARG:HD3 | 1:B:182:TYR:HD2 | 15 | 0.15 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 5 | 0.15 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 13 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 13 | 0.15 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 4 | 0.15 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 4 | 0.15 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 4 | 0.15 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 13 | 0.15 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 13 | 0.15 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 13 | 0.15 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 4 | 0.15 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 11 | 0.15 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 4 | 0.15 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 11 | 0.15 |
| (1,1405) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 13 | 0.15 |
| (1,1405) | 1:B:156:ILE:H | 1:B:156:ILE:HG13 | 15 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 2 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 2 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 2 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 2 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 2 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 2 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 18 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 18 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 18 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 18 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 18 | 0.15 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 18 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD21 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD22 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD23 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD21 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD22 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD23 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD21 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD22 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE1 | 1:B:169:LEU:HD23 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD21 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD22 | 9 | 0.15 |
| (1,1331) | 1:B:165:PHE:HE2 | 1:B:169:LEU:HD23 | 9 | 0.15 |
| (1,1302) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,105) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HB3 | 15 | 0.15 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 10 | 0.14 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 10 | 0.14 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 10 | 0.14 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 10 | 0.14 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 10 | 0.14 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 10 | 0.14 |
| (1,856) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 10 | 0.14 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 4 | 0.14 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 4 | 0.14 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 4 | 0.14 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 8 | 0.14 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 8 | 0.14 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 8 | 0.14 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 9 | 0.14 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 9 | 0.14 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 9 | 0.14 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 14 | 0.14 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 14 | 0.14 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 14 | 0.14 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 1 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 1 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 1 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 2 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 2 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 2 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 3 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 3 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 3 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 5 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 5 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 5 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 6 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 6 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 6 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 7 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 7 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 9 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 9 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 9 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 10 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 10 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 10 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 11 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 11 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 11 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 13 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 13 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 13 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 14 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 14 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 14 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 16 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 16 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 16 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 18 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 18 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 18 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 19 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 19 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 19 | 0.14 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 20 | 0.14 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 20 | 0.14 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 20 | 0.14 |
| (1,387) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 10 | 0.14 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 6 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 1 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 1 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 1 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 2 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 2 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 3 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 3 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 3 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 5 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 5 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 5 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 6 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 6 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 6 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 7 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 7 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 7 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 9 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 9 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 9 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 10 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 10 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 10 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 11 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 11 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 11 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 13 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 13 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 13 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 14 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 14 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 14 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 16 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 16 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 16 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 18 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 18 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 18 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 19 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 19 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 19 | 0.14 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 20 | 0.14 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 20 | 0.14 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 20 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG21 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG22 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG23 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD11 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD12 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD13 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD11 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD12 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD13 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD11 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD12 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD13 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG21 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG22 | 10 | 0.14 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG23 | 10 | 0.14 |
| (1,1979) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA3 | 10 | 0.14 |
| (1,1979) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA3 | 10 | 0.14 |
| (1,1979) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA3 | 10 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 4 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 4 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 4 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 8 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 8 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 8 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 9 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 9 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 9 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 14 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 14 | 0.14 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 14 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG21 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG22 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG23 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG21 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG22 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG23 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD11 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD12 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD13 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD11 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD12 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD13 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD11 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD12 | 10 | 0.14 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD13 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1947) | 1:B:177:ILE:HG21 | 1:B:180:GLY:HA3 | 10 | 0.14 |
| (1,1947) | 1:B:177:ILE:HG22 | 1:B:180:GLY:HA3 | 10 | 0.14 |
| (1,1947) | 1:B:177:ILE:HG23 | 1:B:180:GLY:HA3 | 10 | 0.14 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 18 | 0.14 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 6 | 0.14 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 18 | 0.14 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 16 | 0.14 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 14 | 0.14 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 14 | 0.14 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 14 | 0.14 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 14 | 0.14 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 14 | 0.14 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 14 | 0.14 |
| (1,1336) | 1:B:173:HIS:HD2 | 1:B:172:SER:HB3 | 11 | 0.14 |
| (1,1307) | 1:B:165:PHE:HA | 1:B:168:SER:HB2 | 13 | 0.14 |
| (2,30) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 10 | 0.13 |
| (2,26) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 10 | 0.13 |
| (1,970) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 11 | 0.13 |
| (1,96) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HB2 | 6 | 0.13 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD11 | 11 | 0.13 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD12 | 11 | 0.13 |
| (1,941) | 1:B:155:GLY:HA3 | 1:B:156:ILE:HD13 | 11 | 0.13 |
| (1,856) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 5 | 0.13 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 6 | 0.13 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 6 | 0.13 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 6 | 0.13 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 17 | 0.13 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 17 | 0.13 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 17 | 0.13 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 4 | 0.13 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 4 | 0.13 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 4 | 0.13 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 8 | 0.13 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 8 | 0.13 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 8 | 0.13 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 12 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 12 | 0.13 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 12 | 0.13 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 15 | 0.13 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 15 | 0.13 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 15 | 0.13 |
| (1,732) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 17 | 0.13 |
| (1,732) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 17 | 0.13 |
| (1,732) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 17 | 0.13 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 6 | 0.13 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 6 | 0.13 |
| (1,45) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 6 | 0.13 |
| (1,387) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 5 | 0.13 |
| (1,366) | 1:B:185:ARG:HD3 | 1:B:181:ILE:HG21 | 15 | 0.13 |
| (1,366) | 1:B:185:ARG:HD3 | 1:B:181:ILE:HG22 | 15 | 0.13 |
| (1,366) | 1:B:185:ARG:HD3 | 1:B:181:ILE:HG23 | 15 | 0.13 |
| (1,36) | 1:B:158:SER:HB3 | 1:B:159:ALA:H | 16 | 0.13 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 15 | 0.13 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 8 | 0.13 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 8 | 0.13 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 8 | 0.13 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 12 | 0.13 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 12 | 0.13 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 12 | 0.13 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 15 | 0.13 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 15 | 0.13 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 15 | 0.13 |
| (1,262) | 1:B:170:LEU:HD11 | 1:B:170:LEU:H | 17 | 0.13 |
| (1,262) | 1:B:170:LEU:HD12 | 1:B:170:LEU:H | 17 | 0.13 |
| (1,262) | 1:B:170:LEU:HD13 | 1:B:170:LEU:H | 17 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG21 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG22 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HG23 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD11 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD12 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:183:ILE:HD13 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD11 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD12 | 19 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HD13 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD11 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD12 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:187:LEU:HD13 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG21 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG22 | 19 | 0.13 |
| (1,1984) | 1:B:181:ILE:HA | 1:B:181:ILE:HG23 | 19 | 0.13 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 8 | 0.13 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 8 | 0.13 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 8 | 0.13 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 9 | 0.13 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 9 | 0.13 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 9 | 0.13 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 6 | 0.13 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 6 | 0.13 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 6 | 0.13 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 17 | 0.13 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 17 | 0.13 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 17 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG21 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG22 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HG23 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG21 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG22 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HG23 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD11 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD12 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:183:ILE:HD13 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD11 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD12 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:187:LEU:HD13 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD11 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD12 | 19 | 0.13 |
| (1,1952) | 1:B:181:ILE:HA | 1:B:181:ILE:HD13 | 19 | 0.13 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 16 | 0.13 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 5 | 0.13 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 9 | 0.13 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 12 | 0.13 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 16 | 0.13 |
| (1,1464) | 1:B:163:LYS:H | 1:B:163:LYS:HG2 | 9 | 0.13 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 2 | 0.13 |
| (1,1400) | 1:B:156:ILE:H | 1:B:155:GLY:HA3 | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 3 | 0.13 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 3 | 0.13 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 3 | 0.13 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 3 | 0.13 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 3 | 0.13 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 3 | 0.13 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD21 | 5 | 0.13 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD22 | 5 | 0.13 |
| (1,1151) | 1:B:159:ALA:HA | 1:B:162:LEU:HD23 | 5 | 0.13 |
| (2,6) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 13 | 0.12 |
| (2,6) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 13 | 0.12 |
| (2,6) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 13 | 0.12 |
| (2,1) | 1:B:164:VAL:HG21 | 1:B:163:LYS:HD3 | 13 | 0.12 |
| (2,1) | 1:B:164:VAL:HG22 | 1:B:163:LYS:HD3 | 13 | 0.12 |
| (2,1) | 1:B:164:VAL:HG23 | 1:B:163:LYS:HD3 | 13 | 0.12 |
| (1,96) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HB2 | 1 | 0.12 |
| (1,96) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HB2 | 9 | 0.12 |
| (1,96) | 1:B:163:LYS:HD3 | 1:B:163:LYS:HB2 | 14 | 0.12 |
| (1,856) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 18 | 0.12 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 19 | 0.12 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 19 | 0.12 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 19 | 0.12 |
| (1,77) | 1:B:162:LEU:HD21 | 1:B:161:PHE:HD1 | 14 | 0.12 |
| (1,77) | 1:B:162:LEU:HD21 | 1:B:161:PHE:HD2 | 14 | 0.12 |
| (1,77) | 1:B:162:LEU:HD22 | 1:B:161:PHE:HD1 | 14 | 0.12 |
| (1,77) | 1:B:162:LEU:HD22 | 1:B:161:PHE:HD2 | 14 | 0.12 |
| (1,77) | 1:B:162:LEU:HD23 | 1:B:161:PHE:HD1 | 14 | 0.12 |
| (1,77) | 1:B:162:LEU:HD23 | 1:B:161:PHE:HD2 | 14 | 0.12 |
| (1,758) | 1:B:176:ALA:HB1 | 1:B:173:HIS:HD2 | 15 | 0.12 |
| (1,758) | 1:B:176:ALA:HB2 | 1:B:173:HIS:HD2 | 15 | 0.12 |
| (1,758) | 1:B:176:ALA:HB3 | 1:B:173:HIS:HD2 | 15 | 0.12 |
| (1,387) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 18 | 0.12 |
| (1,1982) | 1:B:181:ILE:HG21 | 1:B:184:GLY:HA3 | 3 | 0.12 |
| (1,1982) | 1:B:181:ILE:HG22 | 1:B:184:GLY:HA3 | 3 | 0.12 |
| (1,1982) | 1:B:181:ILE:HG23 | 1:B:184:GLY:HA3 | 3 | 0.12 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 19 | 0.12 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 19 | 0.12 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 19 | 0.12 |
| (1,1925) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 6 | 0.12 |
| (1,1848) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 6 | 0.12 |
| (1,1725) | 1:B:163:LYS:H | 1:B:160:GLU:HA | 19 | 0.12 |
| (1,1698) | 1:B:160:GLU:H | 1:B:158:SER:HB2 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1698) | 1:B:160:GLU:H | 1:B:158:SER:HB2 | 7 | 0.12 |
| (1,1698) | 1:B:160:GLU:H | 1:B:158:SER:HB2 | 18 | 0.12 |
| (1,1691) | 1:B:158:SER:H | 1:B:162:LEU:HG | 4 | 0.12 |
| (1,1654) | 1:B:172:SER:H | 1:B:171:LEU:HB3 | 6 | 0.12 |
| (1,1579) | 1:B:181:ILE:H | 1:B:178:GLY:HA3 | 6 | 0.12 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 11 | 0.12 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 11 | 0.12 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 11 | 0.12 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 11 | 0.12 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 11 | 0.12 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 11 | 0.12 |
| (1,1159) | 1:B:160:GLU:HA | 1:B:163:LYS:HB3 | 19 | 0.12 |
| (2,30) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 1 | 0.11 |
| (2,26) | 1:B:162:LEU:H | 1:B:158:SER:HB2 | 1 | 0.11 |
| (2,14) | 1:B:185:ARG:HA | 1:B:187:LEU:HG | 14 | 0.11 |
| (1,972) | 1:B:160:GLU:HA | 1:B:163:LYS:HG2 | 4 | 0.11 |
| (1,856) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 2 | 0.11 |
| (1,856) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 7 | 0.11 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 1 | 0.11 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 1 | 0.11 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 1 | 0.11 |
| (1,778) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 16 | 0.11 |
| (1,778) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 16 | 0.11 |
| (1,778) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 16 | 0.11 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,773) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,773) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,773) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 19 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,735) | 1:B:170:LEU:HD11 | 1:B:170:LEU:HB3 | 16 | 0.11 |
| (1,735) | 1:B:170:LEU:HD12 | 1:B:170:LEU:HB3 | 16 | 0.11 |
| (1,735) | 1:B:170:LEU:HD13 | 1:B:170:LEU:HB3 | 16 | 0.11 |
| (1,573) | 1:B:163:LYS:HE3 | 1:B:163:LYS:HB3 | 17 | 0.11 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG11 | 14 | 0.11 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG12 | 14 | 0.11 |
| (1,515) | 1:B:160:GLU:HB2 | 1:B:164:VAL:HG13 | 14 | 0.11 |
| (1,387) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 2 | 0.11 |
| (1,387) | 1:B:185:ARG:HG2 | 1:B:185:ARG:HB3 | 7 | 0.11 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 11 | 0.11 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 14 | 0.11 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,303) | 1:B:177:ILE:HG21 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,303) | 1:B:177:ILE:HG22 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,303) | 1:B:177:ILE:HG23 | 1:B:179:LEU:HG | 19 | 0.11 |
| (1,265) | 1:B:170:LEU:HD11 | 1:B:170:LEU:HB3 | 16 | 0.11 |
| (1,265) | 1:B:170:LEU:HD12 | 1:B:170:LEU:HB3 | 16 | 0.11 |
| (1,265) | 1:B:170:LEU:HD13 | 1:B:170:LEU:HB3 | 16 | 0.11 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 1 | 0.11 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 1 | 0.11 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 1 | 0.11 |
| (1,1978) | 1:B:177:ILE:HG21 | 1:B:180:GLY:H | 16 | 0.11 |
| (1,1978) | 1:B:177:ILE:HG22 | 1:B:180:GLY:H | 16 | 0.11 |
| (1,1978) | 1:B:177:ILE:HG23 | 1:B:180:GLY:H | 16 | 0.11 |
| (1,1812) | 1:B:176:ALA:H | 1:B:173:HIS:HD2 | 15 | 0.11 |
| (1,1699) | 1:B:160:GLU:H | 1:B:158:SER:HB3 | 8 | 0.11 |
| (1,1698) | 1:B:160:GLU:H | 1:B:158:SER:HB2 | 20 | 0.11 |
| (1,1689) | 1:B:158:SER:H | 1:B:161:PHE:HD1 | 14 | 0.11 |
| (1,1689) | 1:B:158:SER:H | 1:B:161:PHE:HD2 | 14 | 0.11 |
| (1,1664) | 1:B:156:ILE:H | 1:B:155:GLY:HA2 | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1664) | 1:B:156:ILE:H | 1:B:155:GLY:HA2 | 12 | 0.11 |
| (1,1404) | 1:B:156:ILE:H | 1:B:156:ILE:HG12 | 10 | 0.11 |
| (1,1400) | 1:B:156:ILE:H | 1:B:155:GLY:HA3 | 1 | 0.11 |
| (1,1400) | 1:B:156:ILE:H | 1:B:155:GLY:HA3 | 17 | 0.11 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 8 | 0.11 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 8 | 0.11 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 8 | 0.11 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB1 | 8 | 0.11 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB2 | 8 | 0.11 |
| (1,1340) | 1:B:173:HIS:HD2 | 1:B:176:ALA:HB3 | 8 | 0.11 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG21 | 4 | 0.11 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG22 | 4 | 0.11 |
| (1,1317) | 1:B:157:PHE:HD1 | 1:B:156:ILE:HG23 | 4 | 0.11 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG21 | 4 | 0.11 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG22 | 4 | 0.11 |
| (1,1317) | 1:B:157:PHE:HD2 | 1:B:156:ILE:HG23 | 4 | 0.11 |
| (1,1141) | 1:B:158:SER:HB3 | 1:B:155:GLY:H | 9 | 0.11 |
| (1,1116) | 1:B:188:THR:HB | 1:B:188:THR:HA | 7 | 0.11 |
| (1,1116) | 1:B:188:THR:HB | 1:B:188:THR:HA | 10 | 0.11 |
| (1,1116) | 1:B:188:THR:HB | 1:B:188:THR:HA | 18 | 0.11 |
| (1,111) | 1:B:163:LYS:HE2 | 1:B:159:ALA:HB1 | 16 | 0.11 |
| (1,111) | 1:B:163:LYS:HE2 | 1:B:159:ALA:HB2 | 16 | 0.11 |
| (1,111) | 1:B:163:LYS:HE2 | 1:B:159:ALA:HB3 | 16 | 0.11 |

# 10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found