# Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 07:36 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 2N3J |
| BMRB ID | : | 25645 |
| Title | : | Solution Structure of the alpha-crystallin domain from the redox-sensitive chaperone, HSPB1 |
| Authors | : | Rajagopal, P.; Liu, Y.; Shi, L.; Klevit, R.E. |
| Deposited on | : | 2015-06-03 |

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:

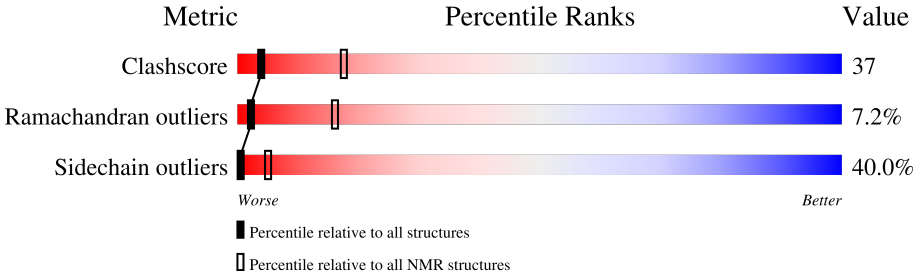
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis | : | 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 20%.

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 | 98 | 21% 39% 13% • 26% |
| 1 | B | 98 | 16% 47% 14% 22% |

# 2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 7 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:94-A:127, A:132-A:170, B:94-B:169 (149) | 0.77 | 7 |

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 3 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3026 atoms, of which 1498 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock protein beta-1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 98 | 1513 | 472 | 749 | 135 | 154 | 3 | 0 |
| 1 | B | 98 | 1513 | 472 | 749 | 135 | 154 | 3 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 79 | MET | - | initiating methionine | UNP P04792 |
| B | 79 | MET | - | initiating methionine | UNP P04792 |

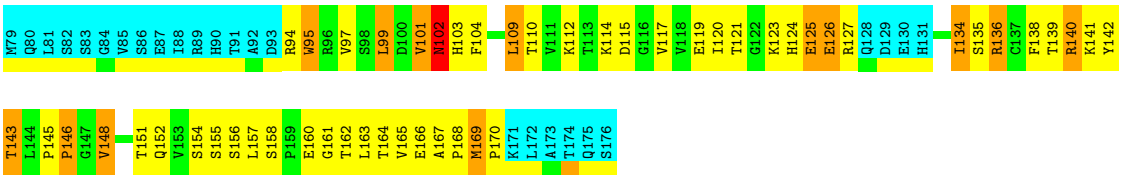
# 4 Residue-property plots (i)

## 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.

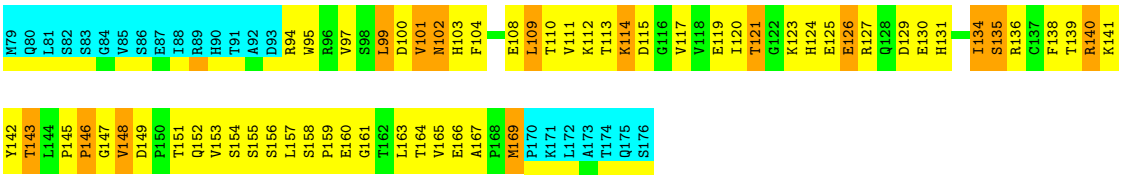
• Molecule 1: Heat shock protein beta-1

Chain A: 21% 39% 13% • 26%




• Molecule 1: Heat shock protein beta-1

Chain B: 16% 47% 14% 22%



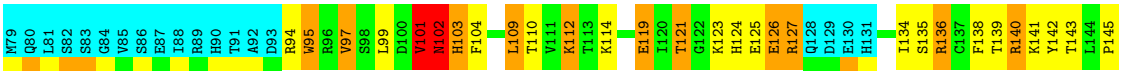

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

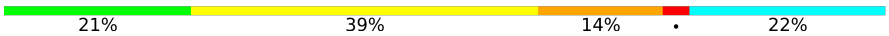
• Molecule 1: Heat shock protein beta-1

Chain A: 28% 30% 15% • 26%



• Molecule 1: Heat shock protein beta-1

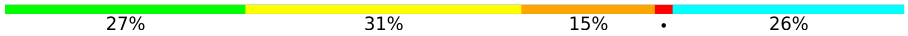
Chain B:

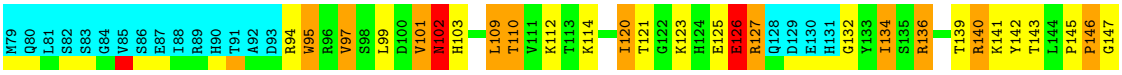


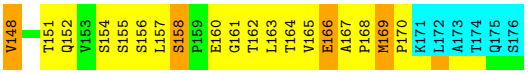
### 4.2.2 Score per residue for model 2

• Molecule 1: Heat shock protein beta-1

Chain A:



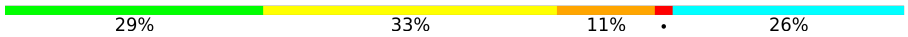

• Molecule 1: Heat shock protein beta-1

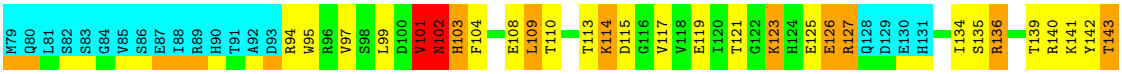
Chain B:

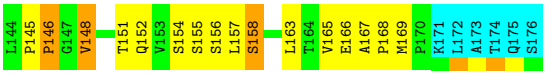
### 4.2.3 Score per residue for model 3

• Molecule 1: Heat shock protein beta-1

Chain A:




• Molecule 1: Heat shock protein beta-1

Chain B: 21% 37% 19% 22%

M79 Q80 L81 S82 S83 G84 V85 S86 E87 I88 R89 H90 T91 A92 D93 R94 W95 R96 V97 S98 L99 D100 V101 N102 H103 F104 A105 E108 L109 T110 V111 K112 T113 K114 V117 V118 E119 I120 T121 G122 K123 H124 E125 E126 R127 Q128 D129 E130 H131 I134 S135 R136 T139 R140 K141 Y142

T143 L144 P145 P146 G147 V148 D149 P150 T151 Q152 V153 S154 S155 S156 L157 S158 P159 E160 G161 T162 L163 T164 V165 E166 A167 P168 M169 P170 K171 L172 A173 T174 Q175 S176

### 4.2.4 Score per residue for model 4

- Molecule 1: Heat shock protein beta-1

Chain A: 27% 35% 12% • 26%

M79 Q80 L81 S82 S83 G84 V85 S86 E87 I88 R89 H90 T91 A92 D93 R94 W95 R96 V97 S98 L99 D100 V101 N102 H103 F104 L109 K112 T113 K114 D115 E119 I120 T121 G122 K123 H124 E125 E126 R127 Q128 D129 E130 H131 G132 Y133 I134 S135 R136 T139 R140 K141 Y142 T143 L144 P145

P146 G147 V148 D149 P150 T151 Q152 V153 S154 S155 S156 L157 S158 G161 T162 L163 T164 V165 E166 A167 P168 M169 P170 K171 L172 A173 T174 Q175 S176

- Molecule 1: Heat shock protein beta-1

Chain B: 21% 36% 18% • 22%

M79 Q80 L81 S82 S83 G84 V85 S86 E87 I88 R89 H90 T91 A92 D93 R94 W95 R96 V97 S98 L99 D100 V101 N102 H103 F104 A105 P106 D107 E108 L109 T110 T113 K114 D115 G116 V117 V118 E119 I120 T121 G122 K123 H124 E125 E126 D129 E130 H131 I134 S135 R136 C137 F138 T139 R140 K141

Y142 T143 L144 P145 P146 G147 V148 T151 Q152 V153 S154 S155 S156 L157 S158 P159 E160 G161 T162 L163 T164 V165 E166 A167 P168 M169 P170 K171 L172 A173 T174 Q175 S176

### 4.2.5 Score per residue for model 5

- Molecule 1: Heat shock protein beta-1

Chain A: 26% 35% 11% • 26%

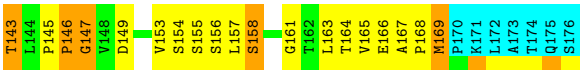
M79 Q80 L81 S82 S83 G84 V85 S86 E87 I88 R89 H90 T91 A92 D93 R94 W95 R96 V97 S98 L99 D100 V101 N102 H103 L109 T110 V111 K112 T113 K114 D115 G116 V117 V118 E119 I120 T121 G122 K123 H124 E125 E126 R127 Q128 D129 E130 H131 G132 Y133 I134 S135 R136 T139 R140 K141 Y142 T143

L144 P145 P146 G147 V148 T151 Q152 V153 S154 S155 S156 L157 S158 G161 T162 L163 T164 V165 E166 A167 P168 M169 P170 K171 L172 A173 T174 Q175 S176

- Molecule 1: Heat shock protein beta-1

Chain B: 21% 40% 16% 22%

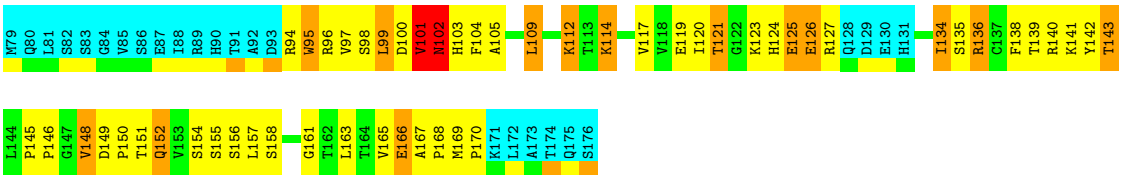
M79 Q80 L81 S82 S83 G84 V85 S86 E87 I88 R89 H90 T91 A92 D93 R94 W95 S98 L99 D100 V101 N102 H103 F104 A105 P106 D107 E108 L109 T110 V111 K112 T113 K114 D115 G116 V117 V118 E119 I120 T121 G122 K123 H124 E125 E126 E130 H131 I134 S135 R136 C137 F138 T139 R140 K141 Y142




### 4.2.6 Score per residue for model 6

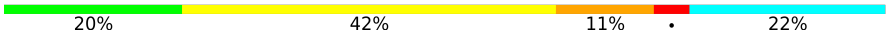
- Molecule 1: Heat shock protein beta-1

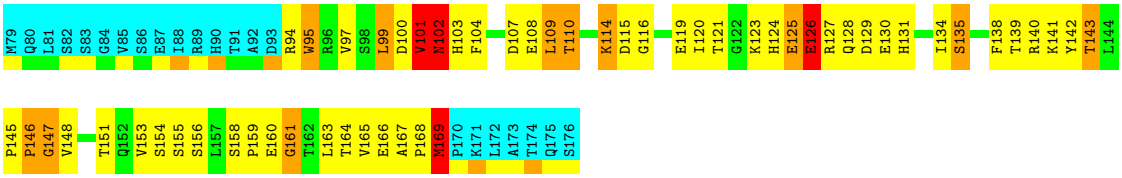
Chain A:




- Molecule 1: Heat shock protein beta-1

Chain B:

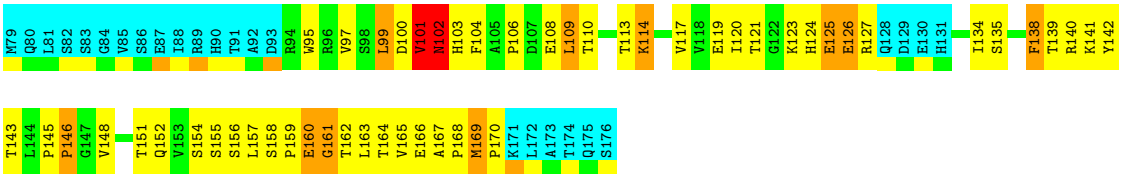



### 4.2.7 Score per residue for model 7 (medoid)

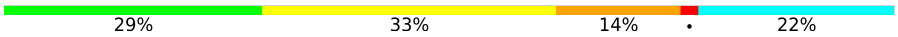
- Molecule 1: Heat shock protein beta-1

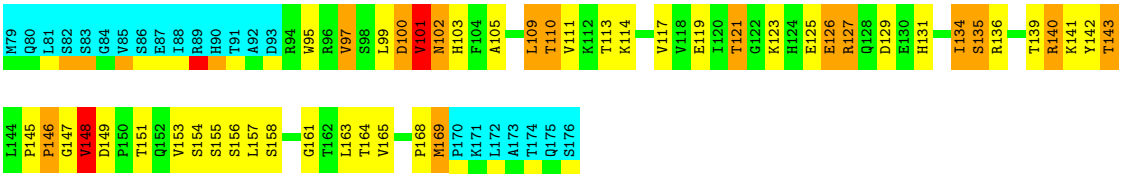
Chain A:




- Molecule 1: Heat shock protein beta-1

Chain B:

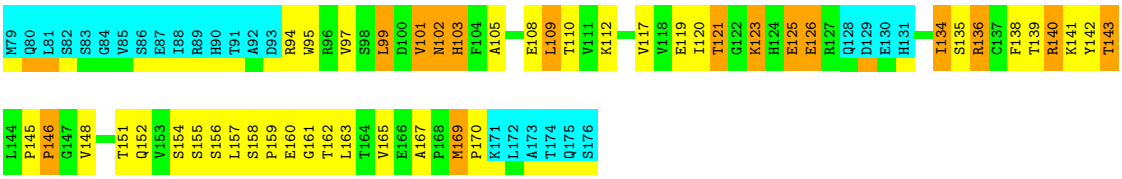


### 4.2.8 Score per residue for model 8

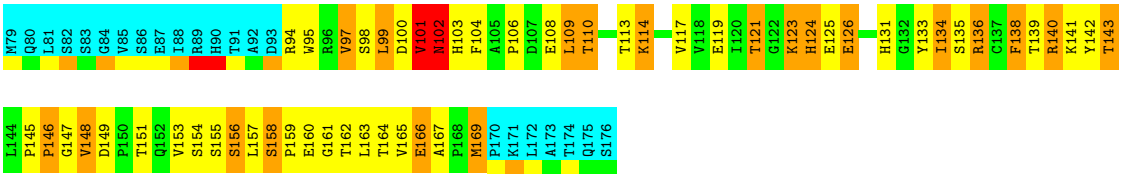
- Molecule 1: Heat shock protein beta-1

Chain A: 27% 33% 15% 26%




- Molecule 1: Heat shock protein beta-1

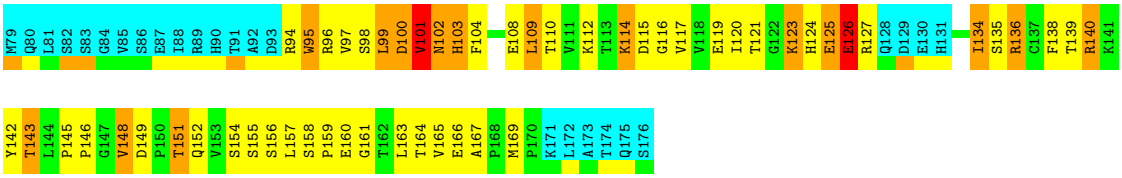
Chain B: 20% 35% 20% • 22%




### 4.2.9 Score per residue for model 9

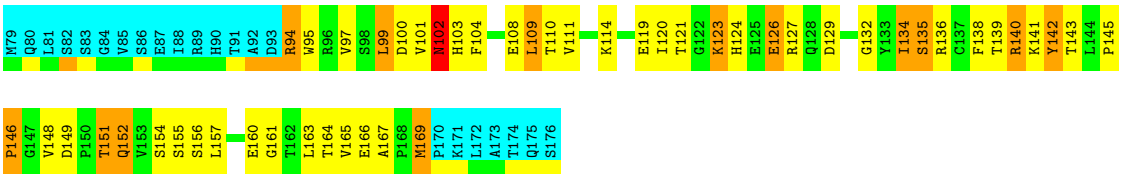
- Molecule 1: Heat shock protein beta-1

Chain A: 18% 39% 15% • 26%




- Molecule 1: Heat shock protein beta-1

Chain B: 27% 37% 13% • 22%




### 4.2.10 Score per residue for model 10

- Molecule 1: Heat shock protein beta-1

Chain A: 20% 40% 14% 26%

M79 Q80 L81 S82 S83 G84 V85 S86 E87 I88 R89 H90 T91 A92 D93 R94 W95 R96 V97 S98 L99 D100 V101 N102 H103 F104 A105 L109 T110 V111 K112 T113 K114 D115 G116 V117 V118 E119 I120 T121 G122 K123 H124 E125 E126 R127 Q128 D129 E130 H131 G132 Y133 I134 S135 R136 T139 R140 K141

Y142 T143 L144 P145 P146 G147 V148 T151 Q152 V153 S154 S155 S156 L157 S158 P159 E160 G161 T162 L163 T164 V165 E166 A167 P168 M169 P170 K171 L172 A173 T174 Q175 S176

- Molecule 1: Heat shock protein beta-1

Chain B: 23% 35% 16% • 22%

M79 Q80 L81 S82 S83 G84 V85 S86 E87 I88 R89 H90 T91 A92 D93 R94 W95 L99 D100 V101 N102 H103 F104 A105 P106 D107 E108 L109 T110 V111 K112 T113 K114 V117 V118 E119 I120 T121 G122 K123 H124 E125 E126 R127 Q128 D129 E130 I134 S135 R136 C137 F138 T139 R140 K141 Y142 T143

L144 P145 P146 G147 V148 D149 P150 T151 Q152 V153 S154 S155 S156 L157 S158 P159 E160 G161 T162 L163 T164 V165 E166 A167 P168 M169 P170 K171 L172 A173 T174 Q175 S176

# 5 Refinement protocol and experimental data overview (i)

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

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

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

| **Software name** | **Classification** | **Version** |
|---|---|---|
| CS-ROSETTA | structure solution | |
| X-PLOR NIH | structure solution | |
| X-PLOR NIH | refinement | |

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

| Chemical shift file(s) | working_cs.cif |
|---|---|
| Number of chemical shift lists | 1 |
| Total number of shifts | 490 |
| Number of shifts mapped to atoms | 490 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 20% |

# 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 | 571 | 565 | 565 | 43±7 |
| 1 | B | 600 | 583 | 583 | 47±6 |
| All | All | 11710 | 11480 | 11480 | 869 |

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 37.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:117:VAL:HG22 | 1:B:143:THR:HG23 | 0.85 | 1.47 | 4 | 6 |
| 1:A:102:ASN:HB3 | 1:A:109:LEU:HD13 | 0.79 | 1.53 | 1 | 4 |
| 1:B:99:LEU:HD22 | 1:B:120:ILE:HG12 | 0.79 | 1.52 | 6 | 3 |
| 1:B:102:ASN:HB3 | 1:B:109:LEU:HD13 | 0.76 | 1.57 | 1 | 4 |
| 1:B:109:LEU:HD22 | 1:B:157:LEU:HD22 | 0.74 | 1.59 | 8 | 9 |
| 1:A:99:LEU:HD23 | 1:A:140:ARG:NE | 0.74 | 1.97 | 7 | 2 |
| 1:B:102:ASN:CB | 1:B:109:LEU:HD13 | 0.73 | 2.14 | 5 | 8 |
| 1:A:102:ASN:HB2 | 1:A:109:LEU:HD13 | 0.71 | 1.61 | 9 | 2 |
| 1:A:109:LEU:HD22 | 1:A:157:LEU:HD22 | 0.70 | 1.61 | 2 | 10 |
| 1:A:99:LEU:HD22 | 1:A:120:ILE:HG13 | 0.69 | 1.62 | 2 | 1 |
| 1:B:102:ASN:HB2 | 1:B:109:LEU:HD13 | 0.69 | 1.63 | 2 | 3 |
| 1:A:127:ARG:CZ | 1:A:127:ARG:HB3 | 0.69 | 2.16 | 2 | 3 |
| 1:B:99:LEU:HD22 | 1:B:120:ILE:HG13 | 0.68 | 1.65 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:117:VAL:HG22 | 1:A:143:THR:HG23 | 0.68 | 1.66 | 8 | 4 |
| 1:A:140:ARG:NH2 | 1:A:142:TYR:CD1 | 0.68 | 2.62 | 8 | 1 |
| 1:B:95:TRP:NE1 | 1:B:97:VAL:HG22 | 0.67 | 2.04 | 1 | 2 |
| 1:A:152:GLN:O | 1:A:167:ALA:HB1 | 0.67 | 1.89 | 2 | 8 |
| 1:A:140:ARG:NH2 | 1:A:142:TYR:CE1 | 0.67 | 2.62 | 8 | 1 |
| 1:B:102:ASN:ND2 | 1:B:102:ASN:H | 0.66 | 1.88 | 9 | 2 |
| 1:A:101:VAL:HG11 | 1:A:138:PHE:CD2 | 0.65 | 2.27 | 7 | 3 |
| 1:A:148:VAL:HA | 1:A:169:MET:SD | 0.65 | 2.31 | 3 | 2 |
| 1:B:102:ASN:OD1 | 1:B:157:LEU:HD11 | 0.65 | 1.91 | 5 | 3 |
| 1:A:95:TRP:CZ3 | 1:A:97:VAL:HG21 | 0.64 | 2.27 | 9 | 4 |
| 1:A:119:GLU:CD | 1:A:141:LYS:NZ | 0.64 | 2.51 | 1 | 2 |
| 1:A:127:ARG:CZ | 1:A:127:ARG:CB | 0.63 | 2.76 | 2 | 2 |
| 1:B:109:LEU:CD2 | 1:B:157:LEU:HD22 | 0.63 | 2.23 | 8 | 4 |
| 1:B:102:ASN:OD1 | 1:B:109:LEU:HD13 | 0.63 | 1.92 | 6 | 3 |
| 1:A:102:ASN:CB | 1:A:109:LEU:HD13 | 0.63 | 2.24 | 1 | 7 |
| 1:A:109:LEU:CD2 | 1:A:157:LEU:HD22 | 0.62 | 2.25 | 7 | 5 |
| 1:A:102:ASN:ND2 | 1:A:102:ASN:H | 0.62 | 1.92 | 1 | 2 |
| 1:A:167:ALA:HB3 | 1:A:169:MET:HE3 | 0.61 | 1.70 | 3 | 1 |
| 1:B:95:TRP:HB2 | 1:B:169:MET:SD | 0.61 | 2.35 | 4 | 3 |
| 1:B:124:HIS:H | 1:B:124:HIS:CD2 | 0.61 | 2.13 | 8 | 1 |
| 1:B:114:LYS:O | 1:B:116:GLY:N | 0.61 | 2.33 | 5 | 3 |
| 1:B:102:ASN:OD1 | 1:B:161:GLY:HA2 | 0.61 | 1.95 | 5 | 3 |
| 1:B:169:MET:SD | 1:B:169:MET:N | 0.60 | 2.74 | 7 | 2 |
| 1:A:99:LEU:HD22 | 1:A:120:ILE:HG12 | 0.60 | 1.73 | 7 | 4 |
| 1:A:166:GLU:O | 1:A:167:ALA:HB2 | 0.60 | 1.95 | 1 | 7 |
| 1:A:102:ASN:OD1 | 1:A:109:LEU:HD13 | 0.60 | 1.96 | 7 | 6 |
| 1:A:119:GLU:CD | 1:A:141:LYS:HZ2 | 0.60 | 2.00 | 7 | 1 |
| 1:A:142:TYR:CE1 | 1:B:132:GLY:HA3 | 0.60 | 2.32 | 9 | 2 |
| 1:A:99:LEU:HD22 | 1:A:120:ILE:CG1 | 0.60 | 2.27 | 4 | 3 |
| 1:B:102:ASN:ND2 | 1:B:102:ASN:N | 0.59 | 2.48 | 9 | 2 |
| 1:B:140:ARG:NH1 | 1:B:142:TYR:OH | 0.59 | 2.30 | 8 | 1 |
| 1:B:102:ASN:ND2 | 1:B:161:GLY:O | 0.59 | 2.35 | 9 | 4 |
| 1:B:114:LYS:O | 1:B:117:VAL:N | 0.59 | 2.34 | 5 | 3 |
| 1:B:99:LEU:HD22 | 1:B:120:ILE:CG1 | 0.59 | 2.28 | 2 | 4 |
| 1:A:95:TRP:NE1 | 1:A:97:VAL:CG2 | 0.59 | 2.65 | 7 | 2 |
| 1:B:152:GLN:O | 1:B:167:ALA:HB1 | 0.59 | 1.96 | 9 | 3 |
| 1:A:95:TRP:NE1 | 1:A:97:VAL:HG22 | 0.59 | 2.13 | 10 | 2 |
| 1:A:134:ILE:O | 1:A:136:ARG:NH2 | 0.59 | 2.35 | 4 | 1 |
| 1:B:130:GLU:N | 1:B:130:GLU:CD | 0.59 | 2.56 | 10 | 1 |
| 1:B:99:LEU:HD23 | 1:B:140:ARG:NE | 0.58 | 2.12 | 4 | 1 |
| 1:B:163:LEU:C | 1:B:163:LEU:HD13 | 0.58 | 2.18 | 2 | 10 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:158:SER:O | 1:A:161:GLY:N | 0.58 | 2.36 | 4 | 2 |
| 1:B:99:LEU:HD23 | 1:B:140:ARG:HH11 | 0.58 | 1.59 | 8 | 1 |
| 1:B:99:LEU:HD21 | 1:B:142:TYR:CE1 | 0.58 | 2.33 | 9 | 1 |
| 1:A:140:ARG:NH2 | 1:A:142:TYR:OH | 0.58 | 2.34 | 7 | 4 |
| 1:B:145:PRO:O | 1:B:147:GLY:N | 0.58 | 2.37 | 10 | 9 |
| 1:A:134:ILE:HD12 | 1:B:140:ARG:NH1 | 0.58 | 2.14 | 2 | 1 |
| 1:A:102:ASN:ND2 | 1:A:102:ASN:N | 0.58 | 2.50 | 1 | 2 |
| 1:A:132:GLY:HA3 | 1:B:142:TYR:CE1 | 0.58 | 2.33 | 2 | 1 |
| 1:A:114:LYS:O | 1:A:116:GLY:N | 0.58 | 2.36 | 9 | 1 |
| 1:B:102:ASN:ND2 | 1:B:105:ALA:O | 0.58 | 2.34 | 3 | 2 |
| 1:A:145:PRO:CD | 1:A:146:PRO:HD3 | 0.57 | 2.29 | 1 | 10 |
| 1:A:102:ASN:O | 1:A:102:ASN:ND2 | 0.57 | 2.34 | 9 | 3 |
| 1:A:99:LEU:HD23 | 1:A:140:ARG:HE | 0.57 | 1.60 | 7 | 1 |
| 1:B:102:ASN:OD1 | 1:B:109:LEU:CD1 | 0.57 | 2.52 | 6 | 2 |
| 1:A:95:TRP:CH2 | 1:A:148:VAL:HG21 | 0.57 | 2.35 | 2 | 3 |
| 1:A:112:LYS:NZ | 1:A:119:GLU:HB2 | 0.57 | 2.14 | 9 | 1 |
| 1:A:165:VAL:O | 1:A:165:VAL:HG23 | 0.57 | 1.99 | 7 | 10 |
| 1:A:140:ARG:NE | 1:A:142:TYR:OH | 0.57 | 2.35 | 4 | 1 |
| 1:A:127:ARG:CB | 1:A:127:ARG:NH1 | 0.57 | 2.68 | 2 | 2 |
| 1:A:145:PRO:HD2 | 1:A:146:PRO:CD | 0.57 | 2.30 | 6 | 1 |
| 1:A:95:TRP:CB | 1:A:169:MET:SD | 0.57 | 2.93 | 5 | 1 |
| 1:A:102:ASN:ND2 | 1:A:161:GLY:O | 0.56 | 2.37 | 1 | 5 |
| 1:B:102:ASN:O | 1:B:102:ASN:ND2 | 0.56 | 2.37 | 2 | 3 |
| 1:B:145:PRO:HD2 | 1:B:146:PRO:CD | 0.56 | 2.30 | 5 | 7 |
| 1:B:108:GLU:OE1 | 1:B:123:LYS:NZ | 0.56 | 2.37 | 3 | 4 |
| 1:A:102:ASN:OD1 | 1:A:161:GLY:HA2 | 0.56 | 2.00 | 8 | 2 |
| 1:B:145:PRO:N | 1:B:146:PRO:CD | 0.56 | 2.68 | 1 | 9 |
| 1:A:140:ARG:NH1 | 1:A:142:TYR:OH | 0.56 | 2.34 | 2 | 2 |
| 1:A:125:GLU:O | 1:A:126:GLU:C | 0.56 | 2.44 | 10 | 8 |
| 1:A:158:SER:HB2 | 1:A:162:THR:HG22 | 0.56 | 1.77 | 4 | 1 |
| 1:B:95:TRP:NE1 | 1:B:97:VAL:CG2 | 0.56 | 2.68 | 8 | 2 |
| 1:A:102:ASN:OD1 | 1:A:109:LEU:HD22 | 0.56 | 1.99 | 6 | 2 |
| 1:A:145:PRO:HD2 | 1:A:146:PRO:HD3 | 0.56 | 1.78 | 9 | 10 |
| 1:A:102:ASN:OD1 | 1:A:157:LEU:HD11 | 0.56 | 1.99 | 8 | 2 |
| 1:A:163:LEU:C | 1:A:163:LEU:HD13 | 0.56 | 2.22 | 2 | 10 |
| 1:A:140:ARG:NH1 | 1:B:133:TYR:O | 0.55 | 2.29 | 8 | 1 |
| 1:B:145:PRO:N | 1:B:146:PRO:HD2 | 0.55 | 2.16 | 2 | 8 |
| 1:A:134:ILE:HD13 | 1:A:136:ARG:NH2 | 0.55 | 2.16 | 6 | 2 |
| 1:B:125:GLU:O | 1:B:126:GLU:C | 0.55 | 2.45 | 7 | 8 |
| 1:A:95:TRP:CZ2 | 1:A:148:VAL:CG2 | 0.55 | 2.89 | 1 | 2 |
| 1:A:99:LEU:CD2 | 1:A:140:ARG:HB3 | 0.55 | 2.31 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:127:ARG:HB2 | 1:B:127:ARG:NH1 | 0.55 | 2.17 | 7 | 1 |
| 1:A:108:GLU:OE1 | 1:A:123:LYS:NZ | 0.54 | 2.38 | 3 | 1 |
| 1:B:126:GLU:HA | 1:B:135:SER:OG | 0.54 | 2.02 | 1 | 6 |
| 1:B:99:LEU:O | 1:B:140:ARG:NH2 | 0.54 | 2.32 | 3 | 2 |
| 1:A:112:LYS:NZ | 1:A:119:GLU:CB | 0.54 | 2.70 | 9 | 2 |
| 1:A:114:LYS:O | 1:A:117:VAL:HG23 | 0.54 | 2.03 | 5 | 3 |
| 1:B:102:ASN:OD1 | 1:B:157:LEU:CD1 | 0.54 | 2.55 | 5 | 1 |
| 1:B:95:TRP:CZ3 | 1:B:97:VAL:HG21 | 0.54 | 2.38 | 6 | 1 |
| 1:B:165:VAL:O | 1:B:165:VAL:HG23 | 0.54 | 2.03 | 4 | 10 |
| 1:B:108:GLU:CD | 1:B:123:LYS:NZ | 0.54 | 2.61 | 5 | 2 |
| 1:A:124:HIS:ND1 | 1:A:125:GLU:N | 0.54 | 2.56 | 6 | 1 |
| 1:B:145:PRO:CD | 1:B:146:PRO:CD | 0.54 | 2.85 | 5 | 6 |
| 1:A:102:ASN:HD22 | 1:A:102:ASN:H | 0.54 | 1.46 | 3 | 1 |
| 1:B:114:LYS:CB | 1:B:114:LYS:NZ | 0.54 | 2.71 | 8 | 1 |
| 1:A:95:TRP:C | 1:A:95:TRP:CD1 | 0.53 | 2.81 | 1 | 1 |
| 1:B:149:ASP:O | 1:B:153:VAL:HG23 | 0.53 | 2.03 | 7 | 6 |
| 1:A:142:TYR:CZ | 1:B:131:HIS:O | 0.53 | 2.61 | 2 | 6 |
| 1:B:102:ASN:C | 1:B:102:ASN:ND2 | 0.53 | 2.62 | 10 | 1 |
| 1:A:100:ASP:C | 1:A:101:VAL:HG22 | 0.53 | 2.23 | 9 | 3 |
| 1:B:148:VAL:CG1 | 1:B:148:VAL:O | 0.53 | 2.56 | 10 | 4 |
| 1:A:142:TYR:CE1 | 1:B:131:HIS:O | 0.53 | 2.61 | 8 | 2 |
| 1:A:102:ASN:OD1 | 1:A:109:LEU:CD1 | 0.53 | 2.56 | 7 | 3 |
| 1:B:102:ASN:C | 1:B:102:ASN:HD22 | 0.53 | 2.07 | 10 | 2 |
| 1:B:145:PRO:CD | 1:B:146:PRO:HD3 | 0.53 | 2.34 | 9 | 4 |
| 1:A:95:TRP:HB3 | 1:A:169:MET:SD | 0.53 | 2.43 | 10 | 1 |
| 1:B:136:ARG:HD3 | 1:B:138:PHE:CE1 | 0.53 | 2.39 | 8 | 1 |
| 1:A:102:ASN:O | 1:A:105:ALA:N | 0.52 | 2.40 | 6 | 2 |
| 1:A:141:LYS:NZ | 1:B:126:GLU:OE1 | 0.52 | 2.42 | 2 | 2 |
| 1:B:119:GLU:HG2 | 1:B:141:LYS:HA | 0.52 | 1.82 | 6 | 2 |
| 1:A:134:ILE:CD1 | 1:A:136:ARG:NH2 | 0.52 | 2.72 | 6 | 1 |
| 1:B:129:ASP:CG | 1:B:130:GLU:N | 0.52 | 2.62 | 10 | 4 |
| 1:B:96:ARG:NH1 | 1:B:96:ARG:HB2 | 0.52 | 2.19 | 4 | 1 |
| 1:A:101:VAL:HG11 | 1:A:138:PHE:CD1 | 0.52 | 2.40 | 1 | 1 |
| 1:B:156:SER:O | 1:B:163:LEU:HD22 | 0.52 | 2.04 | 3 | 4 |
| 1:A:127:ARG:NH1 | 1:A:127:ARG:HB2 | 0.52 | 2.19 | 2 | 2 |
| 1:B:104:PHE:HB2 | 1:B:124:HIS:CE1 | 0.52 | 2.40 | 2 | 1 |
| 1:B:108:GLU:OE2 | 1:B:123:LYS:NZ | 0.52 | 2.41 | 4 | 4 |
| 1:A:112:LYS:NZ | 1:A:121:THR:OG1 | 0.52 | 2.35 | 10 | 4 |
| 1:A:101:VAL:O | 1:A:103:HIS:N | 0.52 | 2.42 | 7 | 5 |
| 1:B:94:ARG:NH1 | 1:B:166:GLU:OE1 | 0.52 | 2.42 | 2 | 3 |
| 1:A:95:TRP:CH2 | 1:A:148:VAL:CG2 | 0.52 | 2.93 | 9 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:124:HIS:O | 1:B:135:SER:CB | 0.52 | 2.58 | 4 | 1 |
| 1:B:127:ARG:CB | 1:B:127:ARG:CZ | 0.52 | 2.88 | 7 | 1 |
| 1:B:153:VAL:HA | 1:B:167:ALA:HB2 | 0.51 | 1.82 | 10 | 5 |
| 1:A:114:LYS:O | 1:A:117:VAL:N | 0.51 | 2.34 | 5 | 1 |
| 1:A:102:ASN:HD22 | 1:A:102:ASN:C | 0.51 | 2.08 | 6 | 1 |
| 1:B:142:TYR:CD1 | 1:B:142:TYR:N | 0.51 | 2.78 | 9 | 5 |
| 1:A:102:ASN:CG | 1:A:109:LEU:HD13 | 0.51 | 2.25 | 5 | 5 |
| 1:B:140:ARG:HB3 | 1:B:140:ARG:CZ | 0.51 | 2.34 | 8 | 1 |
| 1:B:102:ASN:N | 1:B:102:ASN:HD22 | 0.51 | 2.03 | 1 | 2 |
| 1:B:102:ASN:CG | 1:B:109:LEU:HD13 | 0.51 | 2.25 | 6 | 3 |
| 1:A:158:SER:HB3 | 1:A:162:THR:OG1 | 0.51 | 2.05 | 2 | 1 |
| 1:A:159:PRO:C | 1:A:161:GLY:H | 0.51 | 2.09 | 9 | 4 |
| 1:B:145:PRO:HD2 | 1:B:146:PRO:HD3 | 0.51 | 1.83 | 9 | 6 |
| 1:A:127:ARG:N | 1:A:135:SER:OG | 0.51 | 2.44 | 6 | 1 |
| 1:B:101:VAL:C | 1:B:103:HIS:H | 0.51 | 2.08 | 6 | 3 |
| 1:B:143:THR:O | 1:B:145:PRO:HD3 | 0.51 | 2.05 | 1 | 8 |
| 1:B:102:ASN:ND2 | 1:B:102:ASN:C | 0.51 | 2.64 | 2 | 1 |
| 1:B:153:VAL:HG22 | 1:B:167:ALA:CB | 0.51 | 2.36 | 4 | 5 |
| 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 0.50 | 1.83 | 1 | 7 |
| 1:A:114:LYS:NZ | 1:A:119:GLU:OE1 | 0.50 | 2.42 | 5 | 2 |
| 1:B:102:ASN:O | 1:B:104:PHE:N | 0.50 | 2.44 | 3 | 1 |
| 1:A:140:ARG:NH2 | 1:A:141:LYS:C | 0.50 | 2.65 | 8 | 1 |
| 1:A:95:TRP:HB2 | 1:A:169:MET:SD | 0.50 | 2.46 | 5 | 1 |
| 1:A:126:GLU:OE1 | 1:B:141:LYS:NZ | 0.50 | 2.43 | 7 | 3 |
| 1:B:159:PRO:C | 1:B:161:GLY:H | 0.50 | 2.09 | 2 | 6 |
| 1:B:134:ILE:O | 1:B:136:ARG:NH2 | 0.50 | 2.36 | 3 | 1 |
| 1:A:142:TYR:OH | 1:B:131:HIS:O | 0.50 | 2.26 | 7 | 1 |
| 1:A:167:ALA:HB3 | 1:A:169:MET:SD | 0.50 | 2.47 | 8 | 1 |
| 1:A:140:ARG:HA | 1:A:140:ARG:NH1 | 0.50 | 2.22 | 10 | 1 |
| 1:B:100:ASP:C | 1:B:101:VAL:HG22 | 0.50 | 2.26 | 1 | 6 |
| 1:B:114:LYS:NZ | 1:B:119:GLU:OE2 | 0.50 | 2.45 | 3 | 6 |
| 1:B:168:PRO:C | 1:B:169:MET:HG3 | 0.50 | 2.28 | 6 | 1 |
| 1:A:101:VAL:HA | 1:A:103:HIS:CE1 | 0.50 | 2.42 | 9 | 2 |
| 1:A:165:VAL:O | 1:A:165:VAL:CG2 | 0.49 | 2.59 | 4 | 9 |
| 1:B:101:VAL:O | 1:B:103:HIS:N | 0.49 | 2.45 | 6 | 2 |
| 1:B:149:ASP:O | 1:B:153:VAL:CG2 | 0.49 | 2.60 | 7 | 4 |
| 1:A:108:GLU:OE2 | 1:A:123:LYS:NZ | 0.49 | 2.42 | 8 | 2 |
| 1:B:127:ARG:NH1 | 1:B:135:SER:HA | 0.49 | 2.22 | 9 | 1 |
| 1:A:119:GLU:CD | 1:A:141:LYS:HD3 | 0.49 | 2.27 | 10 | 1 |
| 1:A:157:LEU:HD12 | 1:A:158:SER:N | 0.49 | 2.22 | 3 | 1 |
| 1:B:140:ARG:NH2 | 1:B:142:TYR:OH | 0.49 | 2.37 | 7 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:114:LYS:NZ | 1:B:115:ASP:OD1 | 0.49 | 2.45 | 4 | 1 |
| 1:A:104:PHE:O | 1:A:124:HIS:ND1 | 0.49 | 2.34 | 1 | 2 |
| 1:A:101:VAL:HG11 | 1:A:138:PHE:CE2 | 0.49 | 2.42 | 7 | 1 |
| 1:A:95:TRP:CH2 | 1:A:97:VAL:HG21 | 0.49 | 2.42 | 1 | 1 |
| 1:A:169:MET:CB | 1:A:170:PRO:CD | 0.49 | 2.91 | 7 | 1 |
| 1:B:102:ASN:O | 1:B:105:ALA:N | 0.49 | 2.39 | 7 | 3 |
| 1:A:153:VAL:HA | 1:A:167:ALA:HB2 | 0.49 | 1.84 | 5 | 1 |
| 1:A:101:VAL:HG21 | 1:A:138:PHE:CD2 | 0.49 | 2.43 | 8 | 1 |
| 1:A:103:HIS:N | 1:A:161:GLY:HA3 | 0.49 | 2.23 | 10 | 2 |
| 1:A:102:ASN:ND2 | 1:A:161:GLY:C | 0.49 | 2.66 | 1 | 2 |
| 1:B:101:VAL:CG2 | 1:B:140:ARG:CZ | 0.49 | 2.91 | 4 | 1 |
| 1:A:101:VAL:CG1 | 1:A:138:PHE:CD2 | 0.49 | 2.96 | 9 | 2 |
| 1:A:145:PRO:CD | 1:A:146:PRO:CD | 0.48 | 2.90 | 6 | 1 |
| 1:B:94:ARG:NH2 | 1:B:166:GLU:OE2 | 0.48 | 2.40 | 8 | 1 |
| 1:A:142:TYR:CD1 | 1:A:142:TYR:N | 0.48 | 2.80 | 1 | 3 |
| 1:A:95:TRP:CD1 | 1:A:95:TRP:C | 0.48 | 2.86 | 9 | 3 |
| 1:A:95:TRP:CG | 1:A:96:ARG:N | 0.48 | 2.81 | 10 | 1 |
| 1:A:102:ASN:N | 1:A:102:ASN:HD22 | 0.48 | 2.06 | 5 | 2 |
| 1:A:145:PRO:CB | 1:A:146:PRO:HD3 | 0.48 | 2.39 | 1 | 9 |
| 1:B:100:ASP:O | 1:B:101:VAL:HG22 | 0.48 | 2.08 | 4 | 1 |
| 1:B:158:SER:O | 1:B:161:GLY:N | 0.48 | 2.45 | 10 | 3 |
| 1:B:119:GLU:C | 1:B:120:ILE:HD13 | 0.48 | 2.28 | 6 | 1 |
| 1:A:134:ILE:HD13 | 1:A:136:ARG:HH21 | 0.48 | 1.69 | 4 | 1 |
| 1:B:107:ASP:OD1 | 1:B:107:ASP:N | 0.48 | 2.46 | 6 | 1 |
| 1:A:166:GLU:O | 1:A:167:ALA:CB | 0.48 | 2.62 | 1 | 3 |
| 1:A:136:ARG:NH1 | 1:B:138:PHE:CZ | 0.48 | 2.82 | 2 | 1 |
| 1:B:128:GLN:HG2 | 1:B:129:ASP:N | 0.48 | 2.24 | 6 | 1 |
| 1:B:104:PHE:O | 1:B:136:ARG:NH2 | 0.48 | 2.43 | 10 | 1 |
| 1:B:114:LYS:NZ | 1:B:119:GLU:OE1 | 0.48 | 2.41 | 10 | 1 |
| 1:A:101:VAL:C | 1:A:103:HIS:H | 0.48 | 2.11 | 7 | 3 |
| 1:B:115:ASP:O | 1:B:115:ASP:CG | 0.48 | 2.50 | 4 | 1 |
| 1:A:115:ASP:O | 1:A:115:ASP:CG | 0.47 | 2.50 | 5 | 1 |
| 1:A:126:GLU:OE2 | 1:B:141:LYS:NZ | 0.47 | 2.42 | 10 | 4 |
| 1:B:163:LEU:C | 1:B:163:LEU:CD1 | 0.47 | 2.83 | 1 | 9 |
| 1:B:136:ARG:CZ | 1:B:138:PHE:CZ | 0.47 | 2.97 | 4 | 1 |
| 1:B:124:HIS:ND1 | 1:B:126:GLU:O | 0.47 | 2.43 | 9 | 1 |
| 1:B:145:PRO:C | 1:B:147:GLY:N | 0.47 | 2.67 | 7 | 6 |
| 1:B:95:TRP:CB | 1:B:169:MET:SD | 0.47 | 3.02 | 4 | 2 |
| 1:B:148:VAL:O | 1:B:148:VAL:CG1 | 0.47 | 2.63 | 7 | 2 |
| 1:B:166:GLU:O | 1:B:167:ALA:HB2 | 0.47 | 2.10 | 1 | 1 |
| 1:B:134:ILE:O | 1:B:134:ILE:HG23 | 0.47 | 2.09 | 2 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:102:ASN:ND2 | 1:B:102:ASN:O | 0.47 | 2.47 | 10 | 2 |
| 1:A:153:VAL:HG22 | 1:A:167:ALA:CB | 0.47 | 2.40 | 5 | 1 |
| 1:B:168:PRO:O | 1:B:169:MET:O | 0.47 | 2.33 | 6 | 1 |
| 1:B:109:LEU:HD22 | 1:B:157:LEU:CD2 | 0.47 | 2.36 | 8 | 1 |
| 1:B:101:VAL:N | 1:B:103:HIS:CE1 | 0.47 | 2.83 | 1 | 1 |
| 1:B:165:VAL:O | 1:B:165:VAL:CG2 | 0.47 | 2.63 | 1 | 9 |
| 1:B:94:ARG:HH12 | 1:B:166:GLU:CD | 0.47 | 2.14 | 1 | 1 |
| 1:B:102:ASN:CG | 1:B:161:GLY:HA2 | 0.47 | 2.30 | 5 | 3 |
| 1:A:100:ASP:OD1 | 1:A:140:ARG:NH2 | 0.47 | 2.44 | 6 | 1 |
| 1:B:127:ARG:NH2 | 1:B:136:ARG:O | 0.47 | 2.47 | 9 | 1 |
| 1:B:107:ASP:C | 1:B:109:LEU:H | 0.46 | 2.14 | 2 | 1 |
| 1:A:117:VAL:HG13 | 1:A:143:THR:HG23 | 0.46 | 1.86 | 9 | 2 |
| 1:A:134:ILE:HD11 | 1:A:136:ARG:HH11 | 0.46 | 1.68 | 8 | 1 |
| 1:B:124:HIS:CD2 | 1:B:136:ARG:H | 0.46 | 2.27 | 8 | 1 |
| 1:A:124:HIS:ND1 | 1:A:127:ARG:HG2 | 0.46 | 2.26 | 9 | 2 |
| 1:B:102:ASN:HD21 | 1:B:105:ALA:C | 0.46 | 2.12 | 3 | 1 |
| 1:A:99:LEU:HD22 | 1:A:120:ILE:HB | 0.46 | 1.86 | 8 | 1 |
| 1:B:119:GLU:O | 1:B:120:ILE:HD12 | 0.46 | 2.11 | 9 | 2 |
| 1:B:109:LEU:HD11 | 1:B:120:ILE:HG23 | 0.46 | 1.88 | 1 | 1 |
| 1:B:100:ASP:C | 1:B:101:VAL:CG2 | 0.46 | 2.84 | 4 | 1 |
| 1:A:117:VAL:HG22 | 1:A:143:THR:CG2 | 0.46 | 2.41 | 10 | 1 |
| 1:A:140:ARG:CZ | 1:A:142:TYR:CZ | 0.46 | 2.99 | 8 | 1 |
| 1:A:123:LYS:O | 1:A:123:LYS:NZ | 0.46 | 2.35 | 9 | 2 |
| 1:B:124:HIS:CD2 | 1:B:127:ARG:CZ | 0.46 | 2.99 | 10 | 1 |
| 1:A:95:TRP:CZ3 | 1:A:97:VAL:CG2 | 0.46 | 2.99 | 2 | 3 |
| 1:A:109:LEU:HD22 | 1:A:157:LEU:CD2 | 0.46 | 2.35 | 2 | 3 |
| 1:B:123:LYS:NZ | 1:B:123:LYS:O | 0.46 | 2.32 | 8 | 2 |
| 1:B:145:PRO:CB | 1:B:146:PRO:HD3 | 0.46 | 2.41 | 9 | 1 |
| 1:B:95:TRP:CD1 | 1:B:97:VAL:HG22 | 0.46 | 2.46 | 1 | 1 |
| 1:A:94:ARG:NH1 | 1:A:166:GLU:OE1 | 0.45 | 2.49 | 9 | 2 |
| 1:B:95:TRP:CD1 | 1:B:95:TRP:C | 0.45 | 2.90 | 6 | 1 |
| 1:B:149:ASP:OD1 | 1:B:152:GLN:N | 0.45 | 2.45 | 2 | 1 |
| 1:B:108:GLU:CD | 1:B:123:LYS:HZ3 | 0.45 | 2.15 | 5 | 1 |
| 1:B:112:LYS:NZ | 1:B:121:THR:OG1 | 0.45 | 2.40 | 10 | 2 |
| 1:B:134:ILE:HD11 | 1:B:136:ARG:NH2 | 0.45 | 2.25 | 7 | 1 |
| 1:A:102:ASN:CB | 1:A:109:LEU:CD1 | 0.45 | 2.94 | 10 | 1 |
| 1:B:124:HIS:O | 1:B:135:SER:HB3 | 0.45 | 2.11 | 4 | 2 |
| 1:B:112:LYS:NZ | 1:B:119:GLU:HB2 | 0.45 | 2.25 | 1 | 1 |
| 1:A:162:THR:O | 1:A:162:THR:CG2 | 0.45 | 2.65 | 4 | 1 |
| 1:A:108:GLU:N | 1:A:108:GLU:CD | 0.45 | 2.69 | 7 | 1 |
| 1:A:95:TRP:HE1 | 1:A:97:VAL:HG22 | 0.45 | 1.71 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:102:ASN:ND2 | 1:B:161:GLY:CA | 0.45 | 2.79 | 1 | 2 |
| 1:B:111:VAL:HG13 | 1:B:120:ILE:CD1 | 0.45 | 2.42 | 2 | 1 |
| 1:B:109:LEU:HA | 1:B:121:THR:O | 0.45 | 2.11 | 8 | 2 |
| 1:B:102:ASN:HB3 | 1:B:109:LEU:CD1 | 0.45 | 2.41 | 7 | 1 |
| 1:A:169:MET:SD | 1:A:169:MET:N | 0.45 | 2.90 | 1 | 1 |
| 1:A:125:GLU:O | 1:A:126:GLU:HB2 | 0.45 | 2.12 | 9 | 2 |
| 1:A:126:GLU:HA | 1:A:135:SER:OG | 0.45 | 2.12 | 4 | 4 |
| 1:B:109:LEU:HG | 1:B:110:THR:N | 0.45 | 2.27 | 6 | 2 |
| 1:A:119:GLU:HA | 1:A:140:ARG:O | 0.45 | 2.12 | 8 | 1 |
| 1:B:124:HIS:NE2 | 1:B:136:ARG:HG3 | 0.45 | 2.27 | 8 | 1 |
| 1:B:98:SER:HA | 1:B:163:LEU:O | 0.45 | 2.11 | 8 | 3 |
| 1:A:125:GLU:O | 1:A:127:ARG:N | 0.45 | 2.50 | 3 | 1 |
| 1:B:119:GLU:O | 1:B:120:ILE:HD13 | 0.45 | 2.12 | 6 | 1 |
| 1:B:157:LEU:HD12 | 1:B:158:SER:N | 0.45 | 2.27 | 1 | 1 |
| 1:A:99:LEU:HD23 | 1:A:140:ARG:HG3 | 0.45 | 1.89 | 2 | 1 |
| 1:B:104:PHE:O | 1:B:124:HIS:ND1 | 0.45 | 2.34 | 5 | 2 |
| 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 0.44 | 1.89 | 5 | 1 |
| 1:B:103:HIS:N | 1:B:161:GLY:HA3 | 0.44 | 2.28 | 7 | 2 |
| 1:A:162:THR:HG23 | 1:A:162:THR:O | 0.44 | 2.12 | 10 | 2 |
| 1:A:169:MET:HB3 | 1:A:170:PRO:HD2 | 0.44 | 1.90 | 8 | 1 |
| 1:A:163:LEU:C | 1:A:163:LEU:CD1 | 0.44 | 2.85 | 4 | 7 |
| 1:A:114:LYS:NZ | 1:A:119:GLU:OE2 | 0.44 | 2.49 | 7 | 1 |
| 1:A:136:ARG:NH1 | 1:B:138:PHE:CE2 | 0.44 | 2.85 | 9 | 1 |
| 1:B:102:ASN:ND2 | 1:B:161:GLY:C | 0.44 | 2.70 | 9 | 1 |
| 1:A:141:LYS:NZ | 1:B:126:GLU:OE2 | 0.44 | 2.42 | 3 | 1 |
| 1:A:149:ASP:OD1 | 1:A:151:THR:N | 0.44 | 2.51 | 9 | 2 |
| 1:B:99:LEU:CD2 | 1:B:140:ARG:HB2 | 0.44 | 2.42 | 4 | 1 |
| 1:B:102:ASN:C | 1:B:104:PHE:N | 0.44 | 2.69 | 5 | 2 |
| 1:A:102:ASN:ND2 | 1:A:105:ALA:O | 0.44 | 2.45 | 8 | 3 |
| 1:B:147:GLY:O | 1:B:149:ASP:N | 0.44 | 2.51 | 10 | 1 |
| 1:A:141:LYS:HB2 | 1:A:141:LYS:HZ3 | 0.44 | 1.73 | 6 | 1 |
| 1:B:95:TRP:CE2 | 1:B:97:VAL:HG22 | 0.44 | 2.47 | 8 | 1 |
| 1:A:114:LYS:HB3 | 1:A:117:VAL:HB | 0.44 | 1.89 | 6 | 4 |
| 1:A:143:THR:O | 1:A:145:PRO:HD3 | 0.44 | 2.12 | 6 | 2 |
| 1:B:99:LEU:HD23 | 1:B:140:ARG:NH1 | 0.44 | 2.28 | 8 | 1 |
| 1:A:112:LYS:HZ3 | 1:A:119:GLU:HB2 | 0.44 | 1.69 | 9 | 1 |
| 1:B:149:ASP:OD1 | 1:B:151:THR:N | 0.44 | 2.48 | 9 | 1 |
| 1:A:109:LEU:HG | 1:A:110:THR:N | 0.43 | 2.27 | 2 | 1 |
| 1:A:140:ARG:NH2 | 1:A:141:LYS:O | 0.43 | 2.46 | 8 | 1 |
| 1:A:140:ARG:CZ | 1:A:140:ARG:HB3 | 0.43 | 2.43 | 2 | 1 |
| 1:B:149:ASP:OD1 | 1:B:149:ASP:N | 0.43 | 2.49 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:95:TRP:CZ2 | 1:A:165:VAL:HG23 | 0.43 | 2.49 | 2 | 1 |
| 1:A:102:ASN:OD1 | 1:A:161:GLY:CA | 0.43 | 2.67 | 8 | 2 |
| 1:A:167:ALA:HB3 | 1:A:169:MET:CE | 0.43 | 2.42 | 3 | 1 |
| 1:B:104:PHE:CE2 | 1:B:136:ARG:NH2 | 0.43 | 2.86 | 8 | 1 |
| 1:A:140:ARG:NH2 | 1:B:131:HIS:ND1 | 0.43 | 2.66 | 4 | 1 |
| 1:B:104:PHE:CD2 | 1:B:136:ARG:NH2 | 0.43 | 2.86 | 8 | 1 |
| 1:A:96:ARG:CZ | 1:A:96:ARG:HB3 | 0.43 | 2.44 | 9 | 1 |
| 1:A:102:ASN:HB3 | 1:A:109:LEU:CD1 | 0.43 | 2.43 | 10 | 1 |
| 1:A:101:VAL:C | 1:A:103:HIS:N | 0.43 | 2.70 | 6 | 1 |
| 1:A:102:ASN:ND2 | 1:A:102:ASN:O | 0.43 | 2.51 | 8 | 1 |
| 1:A:140:ARG:NH2 | 1:A:141:LYS:N | 0.43 | 2.66 | 8 | 1 |
| 1:A:140:ARG:CZ | 1:A:142:TYR:CE1 | 0.43 | 3.01 | 8 | 1 |
| 1:B:140:ARG:CZ | 1:B:140:ARG:CB | 0.43 | 2.97 | 8 | 1 |
| 1:A:100:ASP:O | 1:A:101:VAL:HG22 | 0.43 | 2.14 | 9 | 1 |
| 1:B:102:ASN:OD1 | 1:B:157:LEU:HD13 | 0.43 | 2.13 | 9 | 2 |
| 1:B:103:HIS:ND1 | 1:B:103:HIS:N | 0.43 | 2.67 | 4 | 1 |
| 1:B:134:ILE:HD11 | 1:B:136:ARG:NH1 | 0.43 | 2.29 | 9 | 1 |
| 1:A:141:LYS:NZ | 1:A:141:LYS:HB2 | 0.43 | 2.28 | 1 | 1 |
| 1:A:102:ASN:ND2 | 1:A:102:ASN:C | 0.43 | 2.73 | 6 | 1 |
| 1:B:104:PHE:HB3 | 1:B:136:ARG:CZ | 0.43 | 2.44 | 10 | 1 |
| 1:A:134:ILE:HA | 1:B:139:THR:O | 0.42 | 2.13 | 4 | 1 |
| 1:A:94:ARG:NH2 | 1:A:166:GLU:OE2 | 0.42 | 2.44 | 2 | 1 |
| 1:B:117:VAL:HG13 | 1:B:143:THR:HG23 | 0.42 | 1.89 | 5 | 1 |
| 1:B:119:GLU:HG2 | 1:B:141:LYS:CB | 0.42 | 2.45 | 4 | 1 |
| 1:A:95:TRP:O | 1:A:166:GLU:HA | 0.42 | 2.13 | 7 | 1 |
| 1:B:136:ARG:O | 1:B:136:ARG:NE | 0.42 | 2.48 | 10 | 1 |
| 1:A:149:ASP:OD2 | 1:A:152:GLN:N | 0.42 | 2.45 | 1 | 1 |
| 1:B:160:GLU:H | 1:B:160:GLU:CD | 0.42 | 2.18 | 1 | 1 |
| 1:B:101:VAL:C | 1:B:103:HIS:N | 0.42 | 2.73 | 6 | 1 |
| 1:A:127:ARG:O | 1:A:134:ILE:N | 0.42 | 2.47 | 9 | 1 |
| 1:A:133:TYR:O | 1:B:141:LYS:N | 0.42 | 2.46 | 10 | 1 |
| 1:A:104:PHE:CE2 | 1:A:136:ARG:NH2 | 0.42 | 2.88 | 1 | 1 |
| 1:A:169:MET:CB | 1:A:170:PRO:HD2 | 0.42 | 2.45 | 8 | 1 |
| 1:B:95:TRP:N | 1:B:167:ALA:O | 0.42 | 2.52 | 2 | 1 |
| 1:B:157:LEU:HD12 | 1:B:158:SER:H | 0.42 | 1.75 | 8 | 1 |
| 1:B:142:TYR:N | 1:B:142:TYR:CD1 | 0.42 | 2.88 | 3 | 1 |
| 1:A:124:HIS:HB3 | 1:A:127:ARG:NH2 | 0.42 | 2.30 | 7 | 1 |
| 1:A:140:ARG:HH22 | 1:A:141:LYS:C | 0.42 | 2.18 | 8 | 1 |
| 1:B:104:PHE:HB3 | 1:B:136:ARG:NH1 | 0.42 | 2.30 | 10 | 1 |
| 1:B:127:ARG:NH1 | 1:B:127:ARG:CB | 0.41 | 2.82 | 7 | 1 |
| 1:A:140:ARG:NE | 1:A:142:TYR:CZ | 0.41 | 2.88 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:95:TRP:CB | 1:B:169:MET:HG2 | 0.41 | 2.45 | 8 | 1 |
| 1:A:124:HIS:CD2 | 1:A:127:ARG:HG3 | 0.41 | 2.50 | 10 | 1 |
| 1:A:101:VAL:N | 1:A:103:HIS:CE1 | 0.41 | 2.88 | 3 | 1 |
| 1:B:145:PRO:C | 1:B:147:GLY:H | 0.41 | 2.18 | 3 | 1 |
| 1:B:158:SER:HB2 | 1:B:162:THR:CG2 | 0.41 | 2.45 | 8 | 1 |
| 1:B:108:GLU:HB3 | 1:B:123:LYS:O | 0.41 | 2.15 | 10 | 1 |
| 1:A:99:LEU:HD23 | 1:A:140:ARG:HD3 | 0.41 | 1.93 | 4 | 1 |
| 1:B:117:VAL:CG1 | 1:B:141:LYS:HG3 | 0.41 | 2.46 | 7 | 1 |
| 1:A:140:ARG:NH1 | 1:B:134:ILE:HB | 0.41 | 2.30 | 10 | 2 |
| 1:A:135:SER:OG | 1:A:136:ARG:N | 0.41 | 2.54 | 3 | 1 |
| 1:B:95:TRP:O | 1:B:166:GLU:HA | 0.41 | 2.16 | 2 | 1 |
| 1:A:119:GLU:HG2 | 1:A:141:LYS:CB | 0.41 | 2.45 | 3 | 2 |
| 1:B:102:ASN:O | 1:B:102:ASN:CG | 0.41 | 2.58 | 3 | 1 |
| 1:B:148:VAL:O | 1:B:149:ASP:C | 0.41 | 2.59 | 3 | 1 |
| 1:A:158:SER:C | 1:A:160:GLU:N | 0.41 | 2.74 | 2 | 1 |
| 1:A:114:LYS:O | 1:A:115:ASP:C | 0.41 | 2.59 | 4 | 1 |
| 1:A:104:PHE:CZ | 1:A:136:ARG:NH1 | 0.41 | 2.89 | 6 | 1 |
| 1:A:99:LEU:CD2 | 1:A:140:ARG:CB | 0.41 | 2.98 | 8 | 1 |
| 1:A:124:HIS:CD2 | 1:A:127:ARG:CG | 0.41 | 3.03 | 1 | 1 |
| 1:B:114:LYS:O | 1:B:115:ASP:C | 0.41 | 2.59 | 1 | 1 |
| 1:A:102:ASN:HB3 | 1:A:161:GLY:O | 0.41 | 2.15 | 6 | 1 |
| 1:B:100:ASP:CG | 1:B:103:HIS:HE2 | 0.41 | 2.19 | 2 | 1 |
| 1:A:132:GLY:HA3 | 1:B:142:TYR:CZ | 0.41 | 2.50 | 5 | 1 |
| 1:A:160:GLU:O | 1:A:162:THR:N | 0.41 | 2.54 | 7 | 1 |
| 1:B:119:GLU:CD | 1:B:141:LYS:HZ2 | 0.41 | 2.16 | 9 | 1 |
| 1:B:160:GLU:CD | 1:B:160:GLU:N | 0.41 | 2.74 | 9 | 1 |
| 1:A:134:ILE:HD12 | 1:B:140:ARG:CZ | 0.41 | 2.45 | 2 | 1 |
| 1:B:104:PHE:CE1 | 1:B:127:ARG:NH1 | 0.41 | 2.89 | 2 | 2 |
| 1:B:110:THR:N | 1:B:121:THR:O | 0.41 | 2.53 | 7 | 1 |
| 1:A:124:HIS:CG | 1:A:127:ARG:HD3 | 0.41 | 2.51 | 10 | 1 |
| 1:B:102:ASN:HD21 | 1:B:106:PRO:HA | 0.41 | 1.75 | 10 | 1 |
| 1:B:157:LEU:HD12 | 1:B:162:THR:O | 0.41 | 2.16 | 3 | 1 |
| 1:B:157:LEU:HD11 | 1:B:161:GLY:HA2 | 0.41 | 1.91 | 3 | 1 |
| 1:B:114:LYS:O | 1:B:117:VAL:CB | 0.41 | 2.68 | 7 | 1 |
| 1:B:127:ARG:NH1 | 1:B:134:ILE:HG23 | 0.40 | 2.31 | 7 | 1 |
| 1:A:119:GLU:HG2 | 1:A:141:LYS:HA | 0.40 | 1.92 | 8 | 1 |
| 1:A:100:ASP:C | 1:A:101:VAL:CG2 | 0.40 | 2.88 | 9 | 1 |
| 1:B:145:PRO:CD | 1:B:146:PRO:HD2 | 0.40 | 2.46 | 5 | 1 |
| 1:A:141:LYS:HB2 | 1:A:141:LYS:NZ | 0.40 | 2.29 | 6 | 1 |
| 1:B:100:ASP:OD2 | 1:B:103:HIS:NE2 | 0.40 | 2.45 | 7 | 1 |
| 1:A:119:GLU:HG2 | 1:A:141:LYS:HB2 | 0.40 | 1.94 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:124:HIS:CD2 | 1:B:124:HIS:N | 0.40 | 2.82 | 8 | 1 |
| 1:B:124:HIS:O | 1:B:135:SER:OG | 0.40 | 2.35 | 4 | 1 |
| 1:A:95:TRP:CD1 | 1:A:95:TRP:O | 0.40 | 2.74 | 6 | 1 |
| 1:A:149:ASP:OD1 | 1:A:152:GLN:N | 0.40 | 2.49 | 9 | 1 |
| 1:B:144:LEU:C | 1:B:146:PRO:HD2 | 0.40 | 2.37 | 2 | 1 |
| 1:B:136:ARG:HD2 | 1:B:138:PHE:CE2 | 0.40 | 2.51 | 5 | 1 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 73/98 (74%) | 58±2 (80±3%) | 10±2 (13±3%) | 5±1 (7±2%) | 2 | 17 |
| 1 | B | 76/98 (78%) | 61±2 (81±3%) | 9±2 (12±3%) | 6±1 (8±2%) | 2 | 15 |
| All | All | 1490/1960 (76%) | 1197 (80%) | 185 (12%) | 108 (7%) | 2 | 16 |

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 126 | GLU | 10 |
| 1 | B | 146 | PRO | 10 |
| 1 | A | 101 | VAL | 9 |
| 1 | B | 101 | VAL | 9 |
| 1 | B | 126 | GLU | 8 |
| 1 | A | 102 | ASN | 7 |
| 1 | A | 146 | PRO | 7 |
| 1 | B | 102 | ASN | 5 |
| 1 | B | 160 | GLU | 5 |
| 1 | A | 147 | GLY | 4 |
| 1 | A | 160 | GLU | 4 |
| 1 | A | 94 | ARG | 3 |
| 1 | B | 106 | PRO | 3 |
| 1 | B | 115 | ASP | 3 |
| 1 | B | 94 | ARG | 3 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 147 | GLY | 3 |
| 1 | A | 170 | PRO | 2 |
| 1 | B | 169 | MET | 2 |
| 1 | B | 100 | ASP | 2 |
| 1 | B | 148 | VAL | 2 |
| 1 | A | 167 | ALA | 1 |
| 1 | B | 103 | HIS | 1 |
| 1 | A | 150 | PRO | 1 |
| 1 | B | 161 | GLY | 1 |
| 1 | A | 106 | PRO | 1 |
| 1 | A | 161 | GLY | 1 |
| 1 | A | 115 | ASP | 1 |

### 6.3.2 Protein sidechains (i)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 66/88 (75%) | 40±2 (61±4%) | 26±2 (39±4%) | 0 6 |
| 1 | B | 69/88 (78%) | 41±3 (59±4%) | 28±3 (41±4%) | 0 4 |
| All | All | 1350/1760 (77%) | 810 (60%) | 540 (40%) | 0 5 |

All 92 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 102 | ASN | 10 |
| 1 | A | 109 | LEU | 10 |
| 1 | A | 121 | THR | 10 |
| 1 | A | 123 | LYS | 10 |
| 1 | A | 134 | ILE | 10 |
| 1 | A | 139 | THR | 10 |
| 1 | A | 143 | THR | 10 |
| 1 | A | 148 | VAL | 10 |
| 1 | A | 151 | THR | 10 |
| 1 | A | 154 | SER | 10 |
| 1 | A | 156 | SER | 10 |
| 1 | B | 99 | LEU | 10 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 109 | LEU | 10 |
| 1 | B | 121 | THR | 10 |
| 1 | B | 134 | ILE | 10 |
| 1 | B | 135 | SER | 10 |
| 1 | B | 139 | THR | 10 |
| 1 | B | 140 | ARG | 10 |
| 1 | B | 154 | SER | 10 |
| 1 | B | 156 | SER | 10 |
| 1 | B | 164 | THR | 10 |
| 1 | A | 99 | LEU | 9 |
| 1 | A | 136 | ARG | 9 |
| 1 | B | 102 | ASN | 9 |
| 1 | B | 123 | LYS | 9 |
| 1 | B | 143 | THR | 9 |
| 1 | B | 148 | VAL | 9 |
| 1 | B | 151 | THR | 9 |
| 1 | B | 155 | SER | 9 |
| 1 | B | 169 | MET | 9 |
| 1 | A | 155 | SER | 9 |
| 1 | B | 110 | THR | 9 |
| 1 | A | 101 | VAL | 8 |
| 1 | A | 169 | MET | 8 |
| 1 | A | 158 | SER | 8 |
| 1 | B | 158 | SER | 8 |
| 1 | A | 95 | TRP | 7 |
| 1 | A | 97 | VAL | 7 |
| 1 | A | 110 | THR | 7 |
| 1 | A | 114 | LYS | 7 |
| 1 | B | 101 | VAL | 7 |
| 1 | B | 113 | THR | 7 |
| 1 | B | 95 | TRP | 7 |
| 1 | A | 140 | ARG | 6 |
| 1 | A | 164 | THR | 6 |
| 1 | B | 97 | VAL | 6 |
| 1 | B | 129 | ASP | 6 |
| 1 | B | 166 | GLU | 6 |
| 1 | A | 112 | LYS | 5 |
| 1 | A | 135 | SER | 5 |
| 1 | B | 125 | GLU | 5 |
| 1 | B | 138 | PHE | 5 |
| 1 | B | 114 | LYS | 5 |
| 1 | A | 125 | GLU | 5 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 103 | HIS | 4 |
| 1 | A | 127 | ARG | 4 |
| 1 | B | 111 | VAL | 4 |
| 1 | B | 126 | GLU | 4 |
| 1 | B | 130 | GLU | 4 |
| 1 | A | 166 | GLU | 4 |
| 1 | A | 113 | THR | 4 |
| 1 | B | 136 | ARG | 4 |
| 1 | B | 94 | ARG | 3 |
| 1 | B | 103 | HIS | 3 |
| 1 | B | 107 | ASP | 3 |
| 1 | A | 126 | GLU | 3 |
| 1 | B | 112 | LYS | 3 |
| 1 | B | 127 | ARG | 3 |
| 1 | A | 104 | PHE | 3 |
| 1 | A | 115 | ASP | 3 |
| 1 | B | 124 | HIS | 3 |
| 1 | A | 98 | SER | 3 |
| 1 | B | 108 | GLU | 2 |
| 1 | B | 115 | ASP | 2 |
| 1 | B | 149 | ASP | 2 |
| 1 | B | 152 | GLN | 2 |
| 1 | A | 96 | ARG | 2 |
| 1 | B | 100 | ASP | 2 |
| 1 | B | 104 | PHE | 2 |
| 1 | A | 100 | ASP | 2 |
| 1 | A | 119 | GLU | 1 |
| 1 | A | 120 | ILE | 1 |
| 1 | B | 120 | ILE | 1 |
| 1 | A | 162 | THR | 1 |
| 1 | A | 111 | VAL | 1 |
| 1 | A | 149 | ASP | 1 |
| 1 | A | 152 | GLN | 1 |
| 1 | A | 138 | PHE | 1 |
| 1 | B | 142 | TYR | 1 |
| 1 | A | 94 | ARG | 1 |
| 1 | A | 124 | HIS | 1 |
| 1 | B | 128 | GLN | 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 20% for the well-defined parts and 19% 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 | 490 |
| Number of shifts mapped to atoms | 490 |
| 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 |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 90 | 0.41 ± 0.15 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 84 | 0.85 ± 0.25 | Should be applied |
| $^{13}C'$ | 0 | — | None (insufficient data) |
| $^{15}N$ | 77 | -0.46 ± 0.36 | None needed (< 0.5 ppm) |

### 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 20%, i.e. 409 atoms were assigned a chemical shift out of a possible 1997. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 219/729 (30%) | 83/295 (28%) | 72/298 (24%) | 64/136 (47%) |
| Sidechain | 188/1133 (17%) | 118/734 (16%) | 68/356 (19%) | 2/43 (5%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 2/135 (1%) | 1/68 (1%) | 0/60 (0%) | 1/7 (14%) |
| Overall | 409/1997 (20%) | 202/1097 (18%) | 140/714 (20%) | 67/186 (36%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 19%, i.e. 490 atoms were assigned a chemical shift out of a possible 2598. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 269/964 (28%) | 102/390 (26%) | 90/392 (23%) | 77/182 (42%) |
| Sidechain | 219/1478 (15%) | 130/958 (14%) | 86/464 (19%) | 3/56 (5%) |
| Aromatic | 2/156 (1%) | 1/80 (1%) | 0/66 (0%) | 1/10 (10%) |
| Overall | 490/2598 (19%) | 233/1428 (16%) | 176/922 (19%) | 81/248 (33%) |

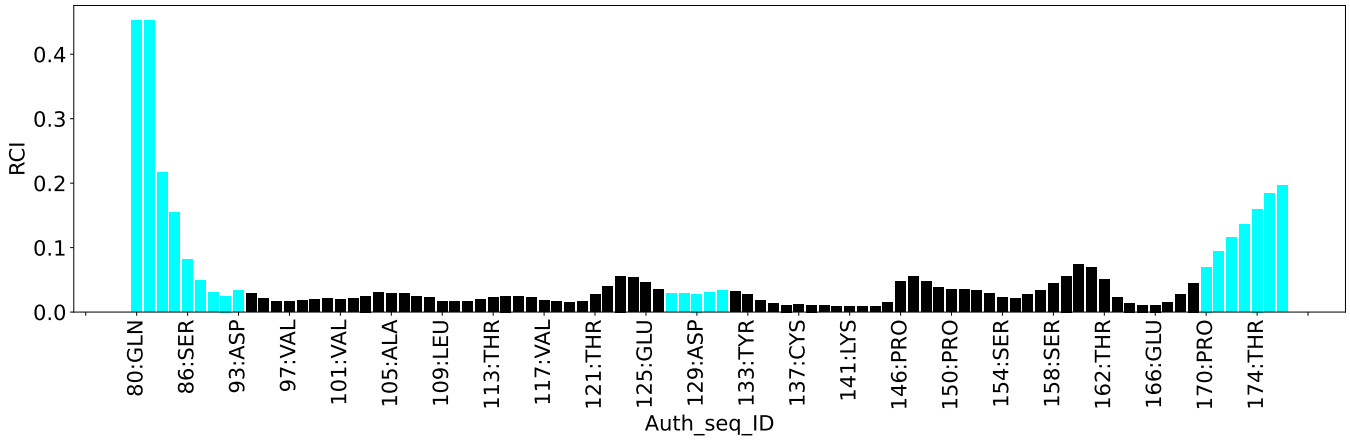
### 7.1.4 Statistically unusual chemical shifts (i)

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 | 4298 |
| Intra-residue (\|i-j\|=0) | 899 |
| Sequential (\|i-j\|=1) | 1094 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 533 |
| Long range (\|i-j\|≥5) | 1507 |
| Inter-chain | 264 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 1 |
| Total dihedral-angle restraints | 230 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 23.1 |
| Number of long range restraints per residue[1] | 7.7 |

[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) | 187.3 | 0.2 |
| 0.2-0.5 (Medium) | 208.2 | 0.5 |
| >0.5 (Large) | 163.3 | 7.17 |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|---|---|---|
| 1.0-10.0 (Small) | 12.6 | 10.0 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

# 9 Distance violation analysis (i)

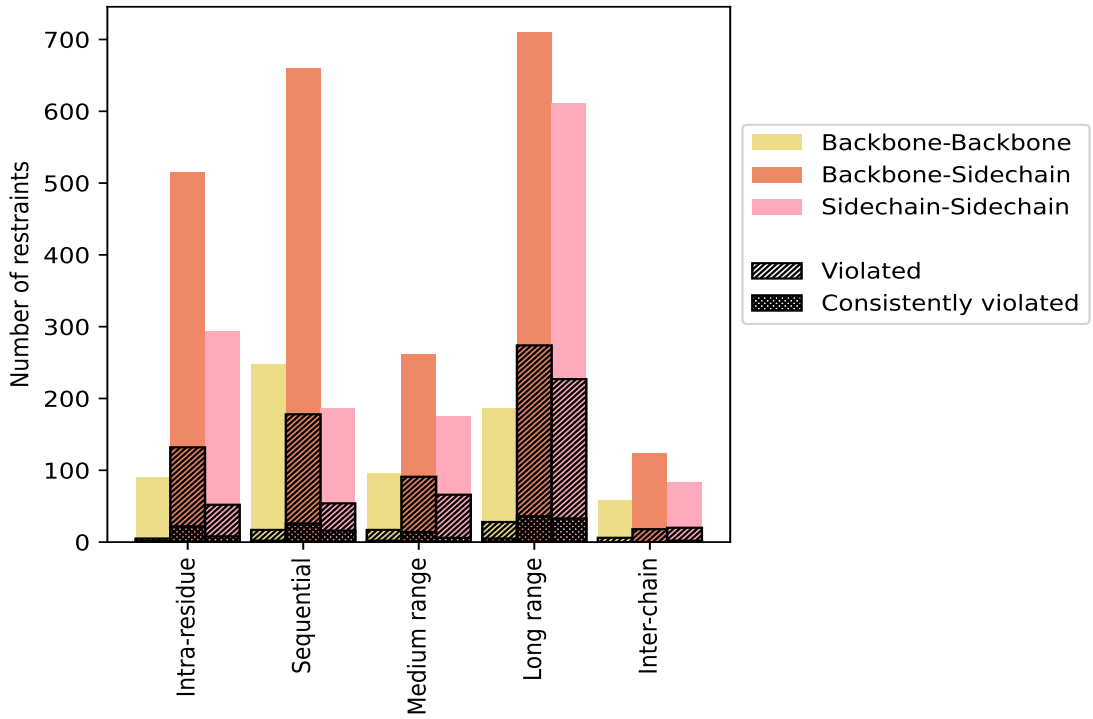
## 9.1 Summary of distance violations (i)

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) | 899 | 20.9 | 189 | 21.0 | 4.4 | 32 | 3.6 | 0.7 |
| Backbone-Backbone | 90 | 2.1 | 5 | 5.6 | 0.1 | 2 | 2.2 | 0.0 |
| Backbone-Sidechain | 515 | 12.0 | 132 | 25.6 | 3.1 | 22 | 4.3 | 0.5 |
| Sidechain-Sidechain | 294 | 6.8 | 52 | 17.7 | 1.2 | 8 | 2.7 | 0.2 |
| Sequential (\|i-j\|=1) | 1094 | 25.5 | 249 | 22.8 | 5.8 | 44 | 4.0 | 1.0 |
| Backbone-Backbone | 248 | 5.8 | 17 | 6.9 | 0.4 | 2 | 0.8 | 0.0 |
| Backbone-Sidechain | 660 | 15.4 | 178 | 27.0 | 4.1 | 26 | 3.9 | 0.6 |
| Sidechain-Sidechain | 186 | 4.3 | 54 | 29.0 | 1.3 | 16 | 8.6 | 0.4 |
| Medium range (\|i-j\|>1 & \|i-j\|<5) | 533 | 12.4 | 174 | 32.6 | 4.0 | 22 | 4.1 | 0.5 |
| Backbone-Backbone | 96 | 2.2 | 17 | 17.7 | 0.4 | 2 | 2.1 | 0.0 |
| Backbone-Sidechain | 262 | 6.1 | 91 | 34.7 | 2.1 | 14 | 5.3 | 0.3 |
| Sidechain-Sidechain | 175 | 4.1 | 66 | 37.7 | 1.5 | 6 | 3.4 | 0.1 |
| Long range (\|i-j\|≥5) | 1507 | 35.1 | 529 | 35.1 | 12.3 | 74 | 4.9 | 1.7 |
| Backbone-Backbone | 186 | 4.3 | 28 | 15.1 | 0.7 | 5 | 2.7 | 0.1 |
| Backbone-Sidechain | 710 | 16.5 | 274 | 38.6 | 6.4 | 36 | 5.1 | 0.8 |
| Sidechain-Sidechain | 611 | 14.2 | 227 | 37.2 | 5.3 | 33 | 5.4 | 0.8 |
| Inter-chain | 264 | 6.1 | 44 | 16.7 | 1.0 | 2 | 0.8 | 0.0 |
| Backbone-Backbone | 58 | 1.3 | 6 | 10.3 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 124 | 2.9 | 18 | 14.5 | 0.4 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 82 | 1.9 | 20 | 24.4 | 0.5 | 2 | 2.4 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 1 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 4298 | 100.0 | 1185 | 27.6 | 27.6 | 174 | 4.0 | 4.0 |
| Backbone-Backbone | 678 | 15.8 | 73 | 10.8 | 1.7 | 11 | 1.6 | 0.3 |
| Backbone-Sidechain | 2271 | 52.8 | 693 | 30.5 | 16.1 | 98 | 4.3 | 2.3 |
| Sidechain-Sidechain | 1349 | 31.4 | 419 | 31.1 | 9.7 | 65 | 4.8 | 1.5 |

[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)

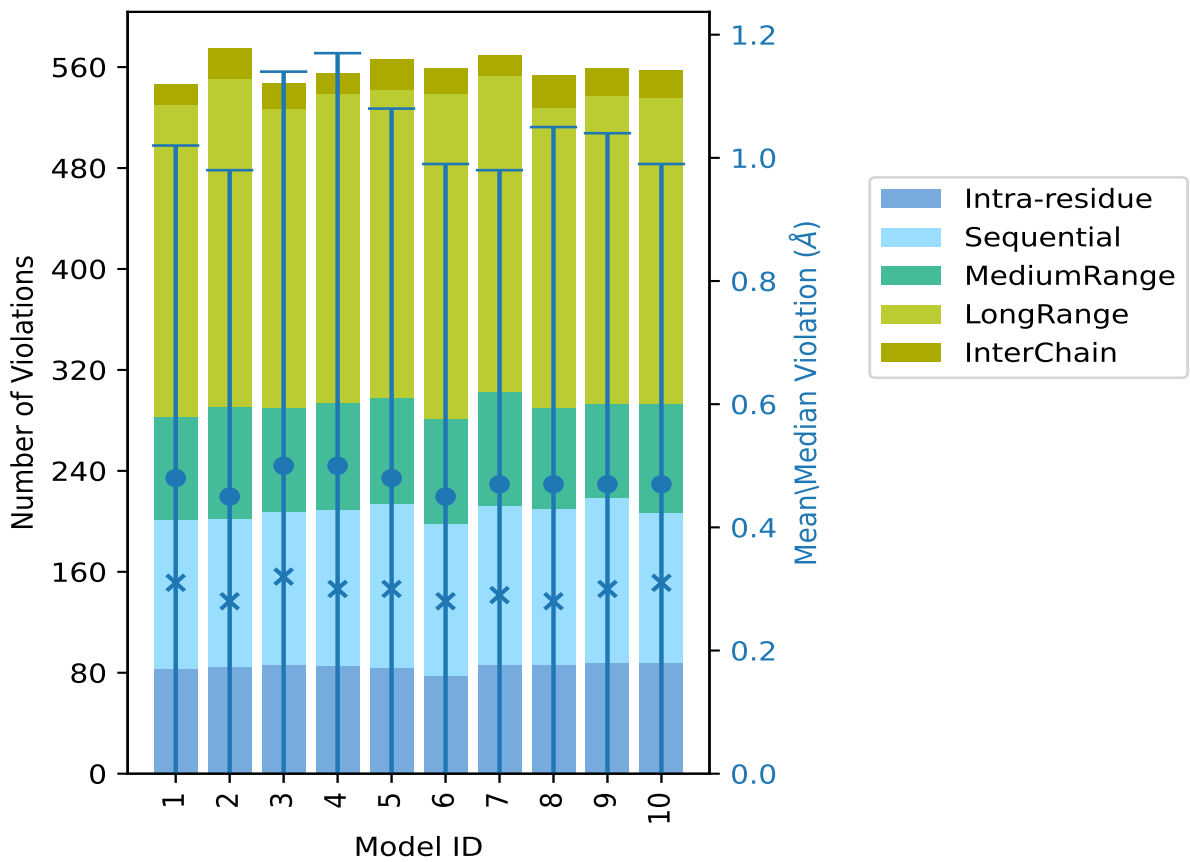
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| 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 | 83 | 118 | 82 | 247 | 16 | 546 | 0.48 | 4.56 | 0.54 | 0.31 |
| 2 | 85 | 117 | 89 | 260 | 24 | 575 | 0.45 | 5.46 | 0.53 | 0.28 |
| 3 | 86 | 122 | 82 | 237 | 20 | 547 | 0.5 | 6.11 | 0.64 | 0.32 |
| 4 | 86 | 123 | 85 | 245 | 16 | 555 | 0.5 | 7.16 | 0.67 | 0.3 |
| 5 | 84 | 130 | 84 | 244 | 24 | 566 | 0.48 | 7.17 | 0.6 | 0.3 |
| 6 | 78 | 120 | 83 | 258 | 20 | 559 | 0.45 | 6.06 | 0.54 | 0.28 |
| 7 | 86 | 126 | 91 | 250 | 16 | 569 | 0.47 | 5.77 | 0.51 | 0.29 |
| 8 | 86 | 124 | 80 | 238 | 26 | 554 | 0.47 | 6.54 | 0.58 | 0.28 |
| 9 | 88 | 131 | 74 | 244 | 22 | 559 | 0.47 | 6.42 | 0.57 | 0.3 |
| 10 | 88 | 119 | 86 | 243 | 22 | 558 | 0.47 | 4.89 | 0.52 | 0.31 |

[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, 3112(IR:710, SQ:845, MR:359, LR:978, IC:220) 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] | % |
| 42 | 63 | 40 | 111 | 8 | 264 | 1 | 10.0 |
| 32 | 29 | 20 | 76 | 6 | 163 | 2 | 20.0 |
| 25 | 24 | 16 | 62 | 4 | 131 | 3 | 30.0 |
| 14 | 16 | 17 | 45 | 4 | 96 | 4 | 40.0 |

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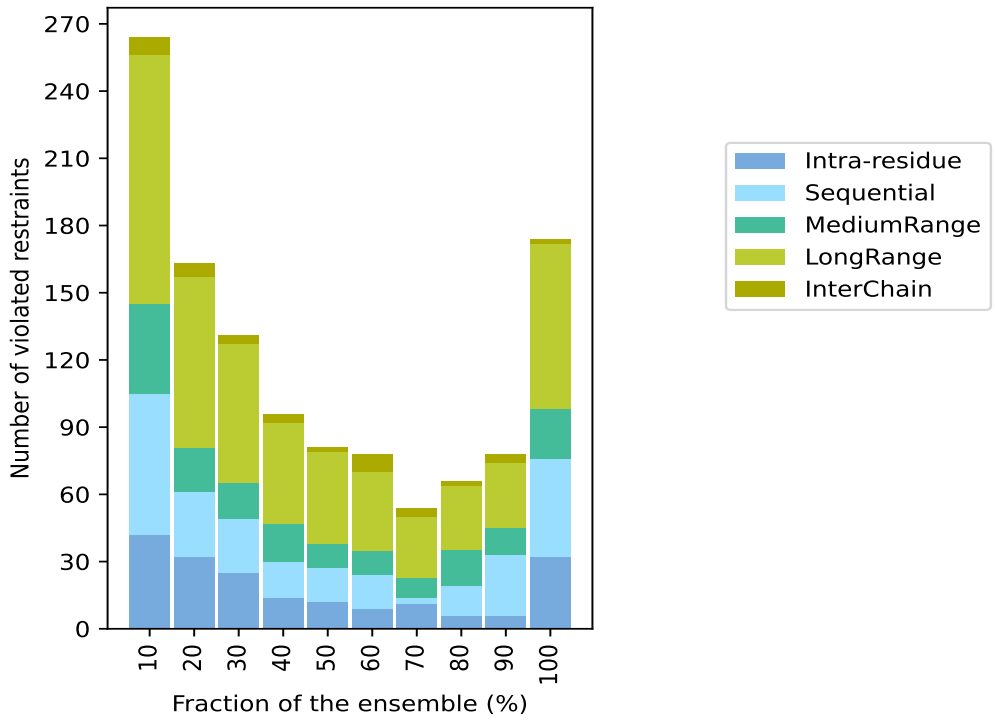
| Number of violated restraints | | | | | | Fraction of the ensemble | |
|---|---|---|---|---|---|---|---|
| IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | Count[6] | % |
| 12 | 15 | 11 | 41 | 2 | 81 | 5 | 50.0 |
| 9 | 15 | 11 | 35 | 8 | 78 | 6 | 60.0 |
| 11 | 3 | 9 | 27 | 4 | 54 | 7 | 70.0 |
| 6 | 13 | 16 | 29 | 2 | 66 | 8 | 80.0 |
| 6 | 27 | 12 | 29 | 4 | 78 | 9 | 90.0 |
| 32 | 44 | 22 | 74 | 2 | 174 | 10 | 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

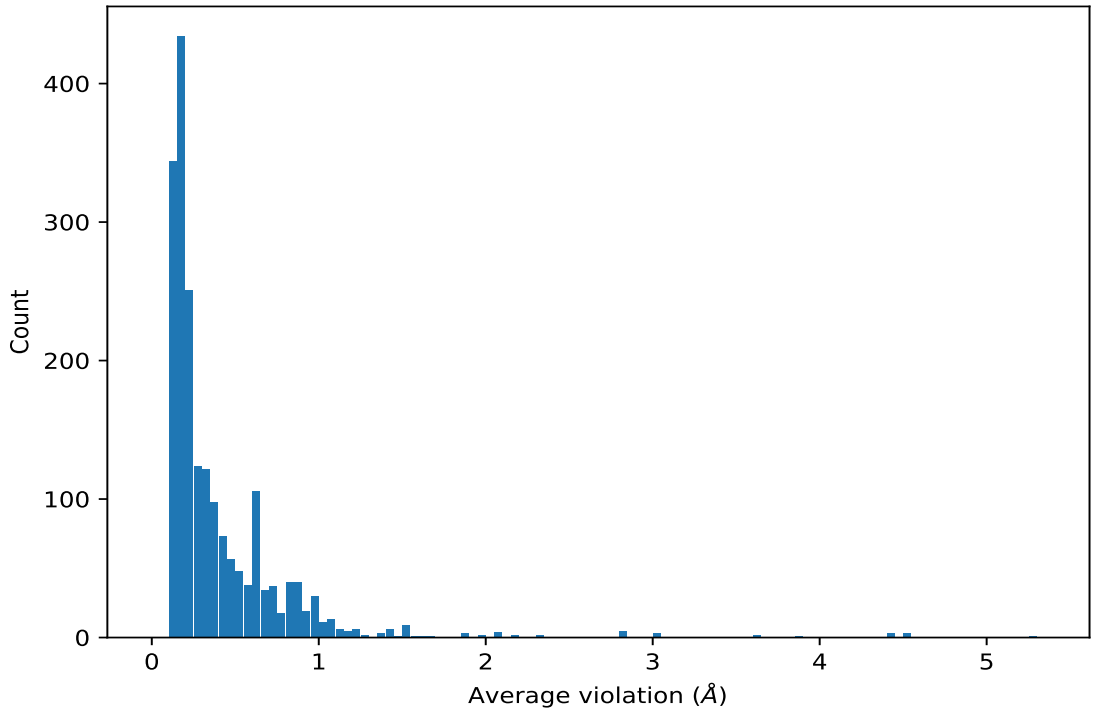
### 9.3.1 Bar graph : Distance violation statistics for the ensemble (i)




## 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) |
|---|---|---|---|---|---|---|
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 10 | 5.28 | 1.15 | 5.49 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 10 | 3.88 | 1.42 | 3.52 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 10 | 3.04 | 1.51 | 3.45 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 10 | 3.04 | 1.51 | 3.45 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 10 | 3.04 | 1.51 | 3.45 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 10 | 1.61 | 0.97 | 1.39 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 10 | 1.55 | 0.06 | 1.56 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 10 | 1.54 | 0.16 | 1.5 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 10 | 1.51 | 0.21 | 1.52 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 10 | 1.37 | 0.37 | 1.46 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 10 | 1.29 | 0.27 | 1.28 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 10 | 1.26 | 0.46 | 1.31 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 10 | 1.24 | 0.29 | 1.34 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 10 | 1.24 | 0.29 | 1.34 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 10 | 1.17 | 0.06 | 1.15 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 10 | 1.17 | 0.06 | 1.15 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 10 | 1.17 | 0.06 | 1.15 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 10 | 1.12 | 0.46 | 1.15 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 10 | 1.12 | 0.46 | 1.15 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 10 | 1.12 | 0.22 | 1.19 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 10 | 1.12 | 0.22 | 1.19 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 10 | 1.09 | 0.09 | 1.08 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 10 | 1.09 | 0.09 | 1.08 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 10 | 1.09 | 0.09 | 1.08 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 10 | 1.06 | 0.25 | 1.11 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 10 | 1.05 | 0.26 | 1.1 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 10 | 1.05 | 0.26 | 1.1 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 10 | 1.05 | 0.26 | 1.1 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 10 | 1.05 | 0.48 | 1.27 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 10 | 1.05 | 0.44 | 1.22 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 10 | 1.04 | 0.19 | 1.04 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 10 | 1.04 | 0.19 | 1.04 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 10 | 1.04 | 0.19 | 1.04 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 10 | 1.01 | 0.24 | 1.17 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 10 | 1.0 | 0.05 | 1.0 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 10 | 1.0 | 0.05 | 1.0 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 10 | 1.0 | 0.05 | 1.0 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 10 | 0.99 | 0.08 | 0.98 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 10 | 0.99 | 0.08 | 0.98 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 10 | 0.99 | 0.08 | 0.98 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 10 | 0.97 | 0.06 | 0.96 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 10 | 0.97 | 0.06 | 0.96 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 10 | 0.97 | 0.06 | 0.96 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 10 | 0.96 | 0.28 | 1.04 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 10 | 0.93 | 0.15 | 0.92 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 10 | 0.93 | 0.32 | 1.0 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 10 | 0.93 | 0.04 | 0.94 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 10 | 0.93 | 0.04 | 0.94 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 10 | 0.91 | 0.19 | 0.98 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 10 | 0.87 | 0.18 | 0.9 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 10 | 0.87 | 0.18 | 0.9 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 10 | 0.87 | 0.18 | 0.9 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 10 | 0.87 | 0.23 | 0.94 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 10 | 0.86 | 0.17 | 0.86 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 10 | 0.86 | 0.1 | 0.9 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 10 | 0.86 | 0.1 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 10 | 0.86 | 0.1 | 0.9 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 10 | 0.84 | 0.29 | 0.92 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 10 | 0.84 | 0.12 | 0.85 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 10 | 0.84 | 0.12 | 0.85 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 10 | 0.83 | 0.26 | 0.94 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 10 | 0.83 | 0.26 | 0.94 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 10 | 0.8 | 0.16 | 0.86 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 10 | 0.8 | 0.23 | 0.79 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 10 | 0.8 | 0.23 | 0.79 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 10 | 0.8 | 0.23 | 0.79 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 10 | 0.79 | 0.21 | 0.76 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 10 | 0.79 | 0.25 | 0.68 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 10 | 0.78 | 0.22 | 0.84 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 10 | 0.78 | 0.13 | 0.74 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 10 | 0.77 | 0.24 | 0.78 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 10 | 0.76 | 0.29 | 0.72 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 10 | 0.76 | 0.29 | 0.72 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 10 | 0.75 | 0.24 | 0.84 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 10 | 0.74 | 0.27 | 0.8 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 10 | 0.74 | 0.27 | 0.8 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 10 | 0.74 | 0.27 | 0.8 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 10 | 0.73 | 0.09 | 0.7 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 10 | 0.73 | 0.09 | 0.7 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 10 | 0.72 | 0.06 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 10 | 0.72 | 0.06 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 10 | 0.72 | 0.06 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 10 | 0.72 | 0.06 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 10 | 0.72 | 0.06 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 10 | 0.72 | 0.06 | 0.74 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 10 | 0.72 | 0.58 | 0.4 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 10 | 0.72 | 0.13 | 0.7 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 10 | 0.72 | 0.13 | 0.7 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 10 | 0.72 | 0.13 | 0.7 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 10 | 0.71 | 0.15 | 0.76 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 10 | 0.71 | 0.15 | 0.76 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 10 | 0.71 | 0.15 | 0.76 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 10 | 0.69 | 0.04 | 0.68 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 10 | 0.69 | 0.38 | 0.55 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 10 | 0.68 | 0.1 | 0.71 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 10 | 0.67 | 0.07 | 0.67 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 10 | 0.67 | 0.07 | 0.67 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 10 | 0.67 | 0.07 | 0.67 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 10 | 0.67 | 0.07 | 0.67 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 10 | 0.67 | 0.07 | 0.67 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 10 | 0.67 | 0.07 | 0.67 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 10 | 0.67 | 0.34 | 0.59 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 10 | 0.67 | 0.34 | 0.59 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 10 | 0.67 | 0.34 | 0.59 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 10 | 0.67 | 0.33 | 0.62 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 10 | 0.66 | 0.18 | 0.7 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 10 | 0.66 | 0.06 | 0.64 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 10 | 0.66 | 0.06 | 0.64 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 10 | 0.65 | 0.13 | 0.62 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 10 | 0.65 | 0.13 | 0.62 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 10 | 0.64 | 0.26 | 0.63 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 10 | 0.64 | 0.15 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 10 | 0.63 | 0.14 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 10 | 0.63 | 0.14 | 0.68 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 10 | 0.63 | 0.08 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 10 | 0.63 | 0.08 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 10 | 0.63 | 0.08 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 10 | 0.63 | 0.08 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 10 | 0.63 | 0.08 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 10 | 0.63 | 0.08 | 0.61 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 10 | 0.62 | 0.12 | 0.66 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 10 | 0.62 | 0.15 | 0.64 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 10 | 0.62 | 0.15 | 0.64 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 10 | 0.62 | 0.15 | 0.64 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 10 | 0.62 | 0.25 | 0.52 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 10 | 0.61 | 0.13 | 0.6 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 10 | 0.61 | 0.13 | 0.6 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 10 | 0.61 | 0.13 | 0.6 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 10 | 0.61 | 0.16 | 0.64 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 10 | 0.61 | 0.16 | 0.64 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 10 | 0.61 | 0.16 | 0.64 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 10 | 0.61 | 0.32 | 0.5 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 10 | 0.6 | 0.09 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 10 | 0.6 | 0.09 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 10 | 0.6 | 0.09 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 10 | 0.6 | 0.09 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 10 | 0.6 | 0.09 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 10 | 0.6 | 0.09 | 0.62 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 10 | 0.6 | 0.18 | 0.67 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 10 | 0.6 | 0.18 | 0.67 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 10 | 0.6 | 0.18 | 0.67 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 10 | 0.6 | 0.1 | 0.6 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 10 | 0.6 | 0.1 | 0.6 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 10 | 0.6 | 0.1 | 0.6 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 10 | 0.6 | 0.2 | 0.6 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 10 | 0.57 | 0.24 | 0.47 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 10 | 0.55 | 0.31 | 0.48 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 10 | 0.55 | 0.14 | 0.58 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 10 | 0.54 | 0.23 | 0.61 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 10 | 0.54 | 0.2 | 0.54 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 10 | 0.54 | 0.08 | 0.53 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 10 | 0.52 | 0.17 | 0.48 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 10 | 0.52 | 0.15 | 0.58 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 10 | 0.51 | 0.17 | 0.46 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 10 | 0.5 | 0.21 | 0.45 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 10 | 0.5 | 0.01 | 0.5 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 10 | 0.49 | 0.02 | 0.48 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 10 | 0.48 | 0.2 | 0.52 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 10 | 0.48 | 0.1 | 0.48 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 10 | 0.48 | 0.2 | 0.54 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 10 | 0.46 | 0.15 | 0.44 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 10 | 0.45 | 0.24 | 0.36 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 10 | 0.45 | 0.24 | 0.36 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 10 | 0.44 | 0.19 | 0.5 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 10 | 0.44 | 0.05 | 0.46 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 10 | 0.43 | 0.04 | 0.42 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 10 | 0.43 | 0.1 | 0.42 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 10 | 0.42 | 0.18 | 0.46 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 10 | 0.42 | 0.05 | 0.43 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 10 | 0.42 | 0.05 | 0.43 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 10 | 0.42 | 0.05 | 0.43 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 10 | 0.41 | 0.07 | 0.42 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 10 | 0.41 | 0.11 | 0.46 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 10 | 0.41 | 0.04 | 0.4 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 10 | 0.41 | 0.04 | 0.41 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 10 | 0.41 | 0.04 | 0.41 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 10 | 0.41 | 0.04 | 0.41 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 10 | 0.39 | 0.02 | 0.4 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 10 | 0.39 | 0.02 | 0.4 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 10 | 0.39 | 0.02 | 0.4 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 10 | 0.39 | 0.1 | 0.4 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 10 | 0.38 | 0.07 | 0.41 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 10 | 0.38 | 0.07 | 0.41 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 10 | 0.38 | 0.07 | 0.41 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 10 | 0.38 | 0.07 | 0.38 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 10 | 0.38 | 0.07 | 0.38 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 10 | 0.38 | 0.07 | 0.38 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 10 | 0.38 | 0.03 | 0.38 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 10 | 0.38 | 0.15 | 0.36 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 10 | 0.38 | 0.12 | 0.36 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 10 | 0.38 | 0.12 | 0.36 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 10 | 0.38 | 0.12 | 0.36 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 10 | 0.38 | 0.13 | 0.36 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 10 | 0.36 | 0.16 | 0.38 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 10 | 0.36 | 0.03 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 10 | 0.36 | 0.09 | 0.33 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 10 | 0.36 | 0.09 | 0.33 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 10 | 0.36 | 0.09 | 0.33 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 10 | 0.36 | 0.09 | 0.33 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 10 | 0.36 | 0.09 | 0.33 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 10 | 0.36 | 0.09 | 0.33 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 10 | 0.36 | 0.2 | 0.24 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 10 | 0.36 | 0.2 | 0.24 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 10 | 0.36 | 0.2 | 0.24 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 10 | 0.35 | 0.08 | 0.35 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 10 | 0.35 | 0.14 | 0.37 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 10 | 0.35 | 0.14 | 0.37 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 10 | 0.35 | 0.1 | 0.36 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 10 | 0.35 | 0.08 | 0.38 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 10 | 0.35 | 0.08 | 0.38 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 10 | 0.35 | 0.16 | 0.34 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 10 | 0.34 | 0.07 | 0.36 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 10 | 0.34 | 0.13 | 0.36 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 10 | 0.34 | 0.13 | 0.36 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 10 | 0.34 | 0.13 | 0.36 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 10 | 0.34 | 0.06 | 0.33 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 10 | 0.33 | 0.03 | 0.34 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 10 | 0.32 | 0.02 | 0.34 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 10 | 0.32 | 0.02 | 0.32 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 10 | 0.32 | 0.04 | 0.32 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 10 | 0.32 | 0.04 | 0.32 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 10 | 0.32 | 0.04 | 0.32 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 10 | 0.32 | 0.06 | 0.31 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 10 | 0.32 | 0.06 | 0.31 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 10 | 0.32 | 0.06 | 0.31 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 10 | 0.32 | 0.07 | 0.29 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 10 | 0.32 | 0.07 | 0.29 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 10 | 0.32 | 0.07 | 0.29 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 10 | 0.3 | 0.03 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 10 | 0.3 | 0.05 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 10 | 0.3 | 0.05 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 10 | 0.3 | 0.05 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 10 | 0.3 | 0.05 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 10 | 0.3 | 0.05 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 10 | 0.3 | 0.05 | 0.3 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 10 | 0.29 | 0.11 | 0.29 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 10 | 0.29 | 0.11 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 10 | 0.29 | 0.11 | 0.29 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 10 | 0.29 | 0.04 | 0.3 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 10 | 0.29 | 0.04 | 0.28 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 10 | 0.29 | 0.04 | 0.28 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 10 | 0.29 | 0.04 | 0.28 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 10 | 0.29 | 0.07 | 0.29 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 10 | 0.29 | 0.07 | 0.29 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 10 | 0.29 | 0.07 | 0.29 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 10 | 0.28 | 0.1 | 0.28 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 10 | 0.27 | 0.03 | 0.28 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 10 | 0.27 | 0.1 | 0.24 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 10 | 0.27 | 0.1 | 0.28 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 10 | 0.26 | 0.08 | 0.29 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 10 | 0.26 | 0.08 | 0.29 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 10 | 0.26 | 0.08 | 0.29 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 10 | 0.25 | 0.1 | 0.24 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 10 | 0.25 | 0.05 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 10 | 0.25 | 0.03 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 10 | 0.25 | 0.03 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 10 | 0.25 | 0.03 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 10 | 0.25 | 0.03 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 10 | 0.25 | 0.03 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 10 | 0.25 | 0.03 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 10 | 0.25 | 0.03 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 10 | 0.25 | 0.03 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 10 | 0.25 | 0.03 | 0.24 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 10 | 0.25 | 0.12 | 0.21 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 10 | 0.24 | 0.04 | 0.24 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 10 | 0.24 | 0.04 | 0.24 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 10 | 0.24 | 0.04 | 0.24 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 10 | 0.24 | 0.02 | 0.25 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 10 | 0.24 | 0.09 | 0.22 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 10 | 0.24 | 0.09 | 0.22 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 10 | 0.24 | 0.09 | 0.22 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 10 | 0.24 | 0.09 | 0.22 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 10 | 0.24 | 0.09 | 0.22 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 10 | 0.24 | 0.09 | 0.22 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 10 | 0.23 | 0.02 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 10 | 0.23 | 0.02 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 10 | 0.23 | 0.02 | 0.24 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 10 | 0.23 | 0.05 | 0.22 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 10 | 0.23 | 0.08 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 10 | 0.23 | 0.08 | 0.22 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 10 | 0.23 | 0.08 | 0.22 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 10 | 0.23 | 0.08 | 0.22 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 10 | 0.23 | 0.08 | 0.22 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 10 | 0.23 | 0.08 | 0.22 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 10 | 0.23 | 0.07 | 0.2 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 10 | 0.23 | 0.06 | 0.23 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 10 | 0.22 | 0.06 | 0.22 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 10 | 0.22 | 0.06 | 0.22 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 10 | 0.22 | 0.06 | 0.22 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 10 | 0.22 | 0.04 | 0.24 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 10 | 0.22 | 0.04 | 0.24 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 10 | 0.22 | 0.04 | 0.24 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 10 | 0.22 | 0.02 | 0.22 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 10 | 0.22 | 0.03 | 0.22 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 10 | 0.22 | 0.03 | 0.22 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 10 | 0.22 | 0.03 | 0.22 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 10 | 0.21 | 0.02 | 0.2 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 10 | 0.21 | 0.02 | 0.21 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 10 | 0.2 | 0.01 | 0.2 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 10 | 0.2 | 0.01 | 0.2 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 10 | 0.2 | 0.06 | 0.2 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 10 | 0.2 | 0.06 | 0.2 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 10 | 0.2 | 0.06 | 0.2 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 10 | 0.2 | 0.02 | 0.2 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 10 | 0.19 | 0.04 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 10 | 0.19 | 0.03 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 10 | 0.19 | 0.03 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 10 | 0.19 | 0.03 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 10 | 0.19 | 0.03 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 10 | 0.19 | 0.03 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 10 | 0.19 | 0.03 | 0.2 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 10 | 0.19 | 0.02 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 10 | 0.19 | 0.02 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 10 | 0.19 | 0.02 | 0.18 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 10 | 0.18 | 0.07 | 0.16 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 10 | 0.18 | 0.07 | 0.16 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 10 | 0.18 | 0.07 | 0.16 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 10 | 0.18 | 0.04 | 0.2 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 10 | 0.18 | 0.05 | 0.19 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 10 | 0.18 | 0.03 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 10 | 0.18 | 0.03 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 10 | 0.18 | 0.03 | 0.17 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 10 | 0.17 | 0.03 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 10 | 0.17 | 0.03 | 0.16 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 10 | 0.16 | 0.01 | 0.16 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 10 | 0.16 | 0.01 | 0.16 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 10 | 0.15 | 0.02 | 0.15 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 10 | 0.15 | 0.03 | 0.15 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 10 | 0.14 | 0.02 | 0.14 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 9 | 3.61 | 1.26 | 3.54 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 9 | 3.61 | 1.26 | 3.54 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 9 | 2.3 | 1.32 | 2.35 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 9 | 2.3 | 1.32 | 2.35 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 9 | 2.08 | 0.97 | 1.99 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 9 | 2.08 | 0.97 | 1.99 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 9 | 2.08 | 0.97 | 1.99 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 9 | 2.08 | 0.97 | 1.99 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 9 | 1.69 | 0.55 | 1.65 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 9 | 1.24 | 0.16 | 1.25 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 9 | 1.07 | 0.63 | 0.67 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 9 | 1.07 | 0.63 | 0.67 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 9 | 1.07 | 0.63 | 0.67 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 9 | 1.0 | 0.47 | 0.95 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 9 | 0.94 | 0.44 | 0.85 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 9 | 0.92 | 0.33 | 0.92 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 9 | 0.91 | 0.5 | 0.79 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 9 | 0.9 | 0.14 | 0.92 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 9 | 0.9 | 0.14 | 0.92 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 9 | 0.89 | 0.28 | 0.76 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 9 | 0.86 | 0.3 | 0.86 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 9 | 0.77 | 0.22 | 0.84 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 9 | 0.73 | 0.07 | 0.76 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 9 | 0.73 | 0.31 | 0.76 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 9 | 0.72 | 0.23 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 9 | 0.72 | 0.23 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 9 | 0.72 | 0.23 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 9 | 0.72 | 0.23 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 9 | 0.72 | 0.23 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 9 | 0.72 | 0.23 | 0.72 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 9 | 0.69 | 0.41 | 0.59 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 9 | 0.69 | 0.41 | 0.59 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 9 | 0.66 | 0.31 | 0.6 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 9 | 0.59 | 0.22 | 0.65 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 9 | 0.59 | 0.22 | 0.65 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 9 | 0.59 | 0.22 | 0.65 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 9 | 0.56 | 0.08 | 0.56 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 9 | 0.55 | 0.19 | 0.58 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 9 | 0.55 | 0.19 | 0.58 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 9 | 0.55 | 0.19 | 0.58 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 9 | 0.54 | 0.16 | 0.56 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 9 | 0.53 | 0.15 | 0.56 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 9 | 0.52 | 0.25 | 0.57 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 9 | 0.52 | 0.25 | 0.57 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 9 | 0.52 | 0.25 | 0.57 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 9 | 0.52 | 0.13 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 9 | 0.52 | 0.13 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 9 | 0.52 | 0.13 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 9 | 0.52 | 0.13 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 9 | 0.52 | 0.13 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 9 | 0.52 | 0.13 | 0.53 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 9 | 0.51 | 0.17 | 0.51 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 9 | 0.51 | 0.17 | 0.51 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 9 | 0.51 | 0.17 | 0.51 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 9 | 0.51 | 0.07 | 0.53 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 9 | 0.48 | 0.06 | 0.45 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 9 | 0.45 | 0.14 | 0.47 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 9 | 0.42 | 0.17 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 9 | 0.39 | 0.19 | 0.42 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 9 | 0.39 | 0.19 | 0.42 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 9 | 0.39 | 0.19 | 0.42 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 9 | 0.38 | 0.13 | 0.38 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 9 | 0.38 | 0.03 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 9 | 0.38 | 0.03 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 9 | 0.38 | 0.03 | 0.39 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 9 | 0.37 | 0.08 | 0.4 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 9 | 0.37 | 0.08 | 0.4 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 9 | 0.37 | 0.08 | 0.4 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 9 | 0.36 | 0.12 | 0.38 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 9 | 0.35 | 0.11 | 0.37 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 9 | 0.35 | 0.14 | 0.37 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 9 | 0.35 | 0.2 | 0.33 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 9 | 0.35 | 0.12 | 0.29 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 9 | 0.35 | 0.13 | 0.34 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 9 | 0.35 | 0.13 | 0.34 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 9 | 0.35 | 0.13 | 0.34 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 9 | 0.34 | 0.19 | 0.23 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 9 | 0.34 | 0.19 | 0.23 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 9 | 0.34 | 0.19 | 0.23 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 9 | 0.34 | 0.09 | 0.27 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 9 | 0.34 | 0.09 | 0.27 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 9 | 0.34 | 0.09 | 0.27 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 9 | 0.33 | 0.15 | 0.38 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 9 | 0.33 | 0.15 | 0.32 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 9 | 0.32 | 0.1 | 0.27 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 9 | 0.32 | 0.1 | 0.27 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 9 | 0.32 | 0.1 | 0.27 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 9 | 0.32 | 0.09 | 0.31 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 9 | 0.32 | 0.09 | 0.31 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 9 | 0.32 | 0.09 | 0.31 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 9 | 0.3 | 0.19 | 0.18 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 9 | 0.3 | 0.19 | 0.18 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 9 | 0.3 | 0.19 | 0.18 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 9 | 0.29 | 0.09 | 0.3 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 9 | 0.29 | 0.09 | 0.3 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 9 | 0.29 | 0.09 | 0.3 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 9 | 0.29 | 0.07 | 0.24 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 9 | 0.29 | 0.07 | 0.24 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 9 | 0.28 | 0.11 | 0.25 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 9 | 0.27 | 0.07 | 0.23 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 9 | 0.27 | 0.06 | 0.26 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 9 | 0.26 | 0.07 | 0.28 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 9 | 0.26 | 0.06 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 9 | 0.26 | 0.06 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 9 | 0.26 | 0.06 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 9 | 0.26 | 0.06 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 9 | 0.26 | 0.06 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 9 | 0.26 | 0.06 | 0.25 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 9 | 0.25 | 0.05 | 0.26 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 9 | 0.25 | 0.15 | 0.15 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 9 | 0.24 | 0.06 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 9 | 0.24 | 0.06 | 0.24 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 9 | 0.24 | 0.07 | 0.24 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 9 | 0.24 | 0.12 | 0.2 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 9 | 0.24 | 0.12 | 0.2 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 9 | 0.24 | 0.12 | 0.2 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 9 | 0.24 | 0.1 | 0.26 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 9 | 0.23 | 0.09 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 9 | 0.23 | 0.09 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 9 | 0.23 | 0.09 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 9 | 0.23 | 0.09 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 9 | 0.23 | 0.09 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 9 | 0.23 | 0.09 | 0.23 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 9 | 0.22 | 0.07 | 0.21 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 9 | 0.22 | 0.04 | 0.23 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 9 | 0.21 | 0.02 | 0.21 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 9 | 0.21 | 0.09 | 0.18 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 9 | 0.21 | 0.09 | 0.18 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 9 | 0.21 | 0.09 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 9 | 0.2 | 0.02 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 9 | 0.2 | 0.02 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 9 | 0.2 | 0.02 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 9 | 0.2 | 0.02 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 9 | 0.2 | 0.02 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 9 | 0.2 | 0.02 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 9 | 0.2 | 0.02 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 9 | 0.2 | 0.02 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 9 | 0.2 | 0.02 | 0.21 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 9 | 0.19 | 0.04 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 9 | 0.19 | 0.04 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 9 | 0.19 | 0.04 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 9 | 0.19 | 0.04 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 9 | 0.19 | 0.04 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 9 | 0.19 | 0.04 | 0.2 |
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 9 | 0.19 | 0.04 | 0.18 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 9 | 0.19 | 0.03 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 9 | 0.19 | 0.03 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 9 | 0.19 | 0.03 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 9 | 0.19 | 0.03 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 9 | 0.19 | 0.03 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 9 | 0.19 | 0.03 | 0.19 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 9 | 0.17 | 0.02 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 9 | 0.17 | 0.04 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 9 | 0.17 | 0.04 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 9 | 0.17 | 0.04 | 0.17 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 9 | 0.16 | 0.04 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 9 | 0.15 | 0.01 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 9 | 0.15 | 0.01 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 9 | 0.15 | 0.01 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 9 | 0.15 | 0.01 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 9 | 0.15 | 0.01 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 9 | 0.15 | 0.01 | 0.15 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 9 | 0.14 | 0.03 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 9 | 0.14 | 0.03 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 9 | 0.14 | 0.03 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 9 | 0.14 | 0.03 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 9 | 0.14 | 0.03 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 9 | 0.14 | 0.03 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 9 | 0.14 | 0.02 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 9 | 0.14 | 0.02 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 9 | 0.14 | 0.02 | 0.14 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 8 | 4.5 | 1.66 | 4.6 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 8 | 4.5 | 1.66 | 4.6 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 8 | 4.5 | 1.66 | 4.6 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 8 | 4.42 | 1.88 | 4.83 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 8 | 4.42 | 1.88 | 4.83 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 8 | 4.42 | 1.88 | 4.83 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 8 | 2.83 | 1.43 | 3.02 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 8 | 2.83 | 1.43 | 3.02 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 8 | 1.99 | 0.41 | 1.83 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 8 | 1.99 | 0.41 | 1.83 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 8 | 1.5 | 0.79 | 1.34 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 8 | 1.5 | 0.79 | 1.34 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 8 | 1.5 | 0.79 | 1.34 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 8 | 1.5 | 0.79 | 1.34 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 8 | 1.4 | 0.52 | 1.62 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 8 | 1.4 | 0.52 | 1.62 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 8 | 1.4 | 0.52 | 1.62 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 8 | 1.1 | 0.39 | 1.16 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 8 | 1.1 | 0.39 | 1.16 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 8 | 1.09 | 0.37 | 1.2 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 8 | 0.91 | 0.5 | 0.94 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 8 | 0.84 | 0.39 | 0.88 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 8 | 0.84 | 0.39 | 0.88 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 8 | 0.7 | 0.19 | 0.78 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 8 | 0.65 | 0.28 | 0.74 |
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 8 | 0.64 | 0.3 | 0.75 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 8 | 0.61 | 0.22 | 0.6 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 8 | 0.61 | 0.22 | 0.6 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 8 | 0.6 | 0.37 | 0.59 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 8 | 0.57 | 0.27 | 0.6 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 8 | 0.57 | 0.27 | 0.6 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 8 | 0.57 | 0.27 | 0.6 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 8 | 0.56 | 0.25 | 0.6 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 8 | 0.56 | 0.25 | 0.6 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 8 | 0.55 | 0.3 | 0.48 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 8 | 0.55 | 0.3 | 0.48 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 8 | 0.55 | 0.3 | 0.48 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 8 | 0.54 | 0.18 | 0.53 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 8 | 0.54 | 0.18 | 0.53 |
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 8 | 0.54 | 0.19 | 0.56 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 8 | 0.52 | 0.28 | 0.42 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 8 | 0.5 | 0.18 | 0.44 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 8 | 0.5 | 0.15 | 0.56 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 8 | 0.49 | 0.13 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 8 | 0.48 | 0.39 | 0.3 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 8 | 0.48 | 0.39 | 0.3 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 8 | 0.48 | 0.39 | 0.3 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 8 | 0.47 | 0.11 | 0.51 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 8 | 0.47 | 0.11 | 0.51 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 8 | 0.47 | 0.11 | 0.51 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 8 | 0.41 | 0.09 | 0.41 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 8 | 0.41 | 0.09 | 0.41 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 8 | 0.41 | 0.09 | 0.41 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 8 | 0.39 | 0.12 | 0.44 |
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 8 | 0.37 | 0.17 | 0.44 |
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 8 | 0.36 | 0.11 | 0.35 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 8 | 0.36 | 0.11 | 0.35 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 8 | 0.36 | 0.11 | 0.35 |
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 8 | 0.34 | 0.11 | 0.34 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 8 | 0.34 | 0.11 | 0.34 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 8 | 0.34 | 0.07 | 0.36 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 8 | 0.32 | 0.13 | 0.34 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 8 | 0.32 | 0.13 | 0.34 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 8 | 0.32 | 0.15 | 0.28 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 8 | 0.32 | 0.15 | 0.28 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 8 | 0.32 | 0.15 | 0.28 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 8 | 0.32 | 0.16 | 0.24 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 8 | 0.32 | 0.16 | 0.24 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 8 | 0.32 | 0.16 | 0.24 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 8 | 0.31 | 0.16 | 0.31 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 8 | 0.31 | 0.06 | 0.3 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 8 | 0.31 | 0.06 | 0.3 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 8 | 0.3 | 0.14 | 0.3 |
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 8 | 0.28 | 0.11 | 0.3 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 8 | 0.27 | 0.14 | 0.21 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 8 | 0.27 | 0.11 | 0.24 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 8 | 0.27 | 0.11 | 0.24 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 8 | 0.27 | 0.11 | 0.24 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 8 | 0.26 | 0.1 | 0.23 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 8 | 0.26 | 0.1 | 0.23 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 8 | 0.25 | 0.07 | 0.28 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 8 | 0.25 | 0.07 | 0.24 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 8 | 0.25 | 0.07 | 0.24 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 8 | 0.24 | 0.13 | 0.2 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 8 | 0.24 | 0.13 | 0.2 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 8 | 0.24 | 0.13 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 8 | 0.24 | 0.06 | 0.26 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 8 | 0.24 | 0.06 | 0.26 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 8 | 0.24 | 0.06 | 0.26 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 8 | 0.22 | 0.06 | 0.23 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 8 | 0.22 | 0.06 | 0.23 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 8 | 0.22 | 0.06 | 0.23 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 8 | 0.22 | 0.06 | 0.23 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 8 | 0.22 | 0.06 | 0.23 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 8 | 0.22 | 0.06 | 0.23 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 8 | 0.22 | 0.05 | 0.22 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 8 | 0.2 | 0.06 | 0.23 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 8 | 0.2 | 0.06 | 0.23 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 8 | 0.2 | 0.06 | 0.23 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 8 | 0.2 | 0.06 | 0.23 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 8 | 0.2 | 0.06 | 0.23 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 8 | 0.2 | 0.06 | 0.23 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 8 | 0.2 | 0.08 | 0.2 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 8 | 0.2 | 0.08 | 0.2 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 8 | 0.2 | 0.08 | 0.2 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 8 | 0.19 | 0.04 | 0.19 |
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 8 | 0.19 | 0.03 | 0.2 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 8 | 0.18 | 0.03 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 8 | 0.18 | 0.03 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 8 | 0.18 | 0.03 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 8 | 0.18 | 0.03 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 8 | 0.18 | 0.03 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 8 | 0.18 | 0.03 | 0.18 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 8 | 0.17 | 0.06 | 0.16 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 8 | 0.17 | 0.06 | 0.16 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 8 | 0.17 | 0.06 | 0.16 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 8 | 0.17 | 0.04 | 0.18 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 8 | 0.17 | 0.04 | 0.18 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 8 | 0.17 | 0.04 | 0.18 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 8 | 0.17 | 0.05 | 0.18 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 8 | 0.17 | 0.05 | 0.18 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 8 | 0.17 | 0.05 | 0.18 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 8 | 0.16 | 0.05 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 8 | 0.16 | 0.05 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 8 | 0.16 | 0.05 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 8 | 0.16 | 0.05 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 8 | 0.16 | 0.05 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 8 | 0.16 | 0.05 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 8 | 0.16 | 0.05 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 8 | 0.16 | 0.05 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 8 | 0.16 | 0.05 | 0.15 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 8 | 0.16 | 0.04 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 8 | 0.16 | 0.04 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 8 | 0.16 | 0.04 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 8 | 0.16 | 0.04 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 8 | 0.16 | 0.04 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 8 | 0.16 | 0.04 | 0.16 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 8 | 0.16 | 0.03 | 0.15 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 8 | 0.16 | 0.03 | 0.15 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 8 | 0.16 | 0.03 | 0.15 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 8 | 0.16 | 0.03 | 0.15 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 8 | 0.16 | 0.03 | 0.15 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 8 | 0.16 | 0.03 | 0.15 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 8 | 0.16 | 0.03 | 0.15 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 8 | 0.16 | 0.03 | 0.15 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 8 | 0.16 | 0.03 | 0.15 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 8 | 0.15 | 0.05 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 8 | 0.15 | 0.05 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 8 | 0.15 | 0.05 | 0.14 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 8 | 0.15 | 0.02 | 0.16 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 8 | 0.15 | 0.04 | 0.16 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 8 | 0.15 | 0.02 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 8 | 0.15 | 0.03 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 8 | 0.15 | 0.03 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 8 | 0.15 | 0.03 | 0.15 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 8 | 0.14 | 0.03 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 8 | 0.14 | 0.03 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 8 | 0.14 | 0.03 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 8 | 0.14 | 0.03 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 8 | 0.14 | 0.03 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 8 | 0.14 | 0.03 | 0.14 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB1 | 7 | 2.8 | 0.93 | 2.74 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB2 | 7 | 2.8 | 0.93 | 2.74 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB3 | 7 | 2.8 | 0.93 | 2.74 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE2 | 7 | 2.18 | 1.2 | 1.67 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE3 | 7 | 2.18 | 1.2 | 1.67 |
| (1,2) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HB3 | 7 | 1.86 | 1.16 | 1.38 |
| (1,2) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HB3 | 7 | 1.86 | 1.16 | 1.38 |
| (1,2) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HB3 | 7 | 1.86 | 1.16 | 1.38 |
| (1,2283) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HB3 | 7 | 1.53 | 0.92 | 1.58 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2283) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HB3 | 7 | 1.53 | 0.92 | 1.58 |
| (1,2283) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HB3 | 7 | 1.53 | 0.92 | 1.58 |
| (1,2061) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 7 | 0.99 | 0.28 | 1.14 |
| (1,2193) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 7 | 0.99 | 0.28 | 1.14 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB1 | 7 | 0.93 | 0.11 | 0.96 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB2 | 7 | 0.93 | 0.11 | 0.96 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB3 | 7 | 0.93 | 0.11 | 0.96 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE1 | 7 | 0.89 | 0.23 | 0.99 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE2 | 7 | 0.89 | 0.23 | 0.99 |
| (1,3566) | 1:B:168:PRO:HD2 | 1:B:169:MET:HA | 7 | 0.76 | 0.31 | 0.84 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE1 | 7 | 0.75 | 0.14 | 0.81 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE2 | 7 | 0.75 | 0.14 | 0.81 |
| (1,4267) | 1:B:167:ALA:H | 1:B:169:MET:H | 7 | 0.73 | 0.33 | 0.65 |
| (1,839) | 1:A:140:ARG:HB2 | 1:A:140:ARG:HD2 | 7 | 0.72 | 0.26 | 0.77 |
| (1,839) | 1:A:140:ARG:HB3 | 1:A:140:ARG:HD2 | 7 | 0.72 | 0.26 | 0.77 |
| (1,1766) | 1:A:149:ASP:H | 1:A:169:MET:HG3 | 7 | 0.68 | 0.54 | 0.54 |
| (1,2282) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HA | 7 | 0.64 | 0.41 | 0.51 |
| (1,2282) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HA | 7 | 0.64 | 0.41 | 0.51 |
| (1,2282) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HA | 7 | 0.64 | 0.41 | 0.51 |
| (1,2322) | 1:B:94:ARG:HB3 | 1:B:167:ALA:HA | 7 | 0.61 | 0.26 | 0.67 |
| (1,2969) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB3 | 7 | 0.58 | 0.21 | 0.57 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG3 | 7 | 0.54 | 0.26 | 0.45 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG2 | 7 | 0.54 | 0.26 | 0.45 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG11 | 7 | 0.52 | 0.32 | 0.39 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG12 | 7 | 0.52 | 0.32 | 0.39 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG13 | 7 | 0.52 | 0.32 | 0.39 |
| (1,1654) | 1:A:134:ILE:H | 1:A:127:ARG:HB2 | 7 | 0.45 | 0.43 | 0.3 |
| (1,2020) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 7 | 0.44 | 0.41 | 0.33 |
| (1,699) | 1:A:125:GLU:HA | 1:A:125:GLU:HG2 | 7 | 0.4 | 0.15 | 0.5 |
| (1,3003) | 1:B:126:GLU:HG2 | 1:B:135:SER:HA | 7 | 0.4 | 0.24 | 0.28 |
| (1,2790) | 1:B:114:LYS:HA | 1:B:114:LYS:HB2 | 7 | 0.38 | 0.13 | 0.44 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD2 | 7 | 0.38 | 0.15 | 0.4 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD3 | 7 | 0.38 | 0.15 | 0.4 |
| (1,2561) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA3 | 7 | 0.34 | 0.22 | 0.2 |
| (1,718) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HB3 | 7 | 0.34 | 0.11 | 0.35 |
| (1,51) | 1:A:95:TRP:HA | 1:A:95:TRP:HB2 | 7 | 0.33 | 0.07 | 0.37 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG11 | 7 | 0.33 | 0.12 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG12 | 7 | 0.33 | 0.12 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG13 | 7 | 0.33 | 0.12 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG11 | 7 | 0.33 | 0.12 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG12 | 7 | 0.33 | 0.12 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG13 | 7 | 0.33 | 0.12 | 0.33 |
| (1,1193) | 1:A:158:SER:HB3 | 1:A:160:GLU:HB3 | 7 | 0.32 | 0.14 | 0.34 |
| (1,1097) | 1:A:154:SER:HB3 | 1:A:155:SER:HA | 7 | 0.3 | 0.08 | 0.28 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD2 | 7 | 0.29 | 0.1 | 0.28 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD3 | 7 | 0.29 | 0.1 | 0.28 |
| (1,1621) | 1:A:129:ASP:H | 1:A:129:ASP:HB2 | 7 | 0.26 | 0.05 | 0.23 |
| (1,2383) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HB3 | 7 | 0.26 | 0.08 | 0.25 |
| (1,102) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HB3 | 7 | 0.26 | 0.07 | 0.28 |
| (1,3295) | 1:B:148:VAL:HG11 | 1:B:170:PRO:HG3 | 7 | 0.24 | 0.03 | 0.25 |
| (1,3295) | 1:B:148:VAL:HG12 | 1:B:170:PRO:HG3 | 7 | 0.24 | 0.03 | 0.25 |
| (1,3295) | 1:B:148:VAL:HG13 | 1:B:170:PRO:HG3 | 7 | 0.24 | 0.03 | 0.25 |
| (1,3726) | 1:B:111:VAL:H | 1:B:110:THR:HB | 7 | 0.22 | 0.07 | 0.24 |
| (1,2783) | 1:B:113:THR:HG21 | 1:B:150:PRO:HB3 | 7 | 0.22 | 0.09 | 0.22 |
| (1,2783) | 1:B:113:THR:HG22 | 1:B:150:PRO:HB3 | 7 | 0.22 | 0.09 | 0.22 |
| (1,2783) | 1:B:113:THR:HG23 | 1:B:150:PRO:HB3 | 7 | 0.22 | 0.09 | 0.22 |
| (1,1168) | 1:A:157:LEU:HD11 | 1:A:161:GLY:HA3 | 7 | 0.21 | 0.05 | 0.19 |
| (1,1168) | 1:A:157:LEU:HD12 | 1:A:161:GLY:HA3 | 7 | 0.21 | 0.05 | 0.19 |
| (1,1168) | 1:A:157:LEU:HD13 | 1:A:161:GLY:HA3 | 7 | 0.21 | 0.05 | 0.19 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD3 | 7 | 0.2 | 0.09 | 0.16 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD2 | 7 | 0.2 | 0.09 | 0.16 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG11 | 7 | 0.19 | 0.06 | 0.19 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG12 | 7 | 0.19 | 0.06 | 0.19 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG13 | 7 | 0.19 | 0.06 | 0.19 |
| (1,3894) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HA | 7 | 0.19 | 0.05 | 0.18 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG21 | 7 | 0.18 | 0.06 | 0.15 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG22 | 7 | 0.18 | 0.06 | 0.15 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG23 | 7 | 0.18 | 0.06 | 0.15 |
| (1,1149) | 1:A:157:LEU:HA | 1:A:163:LEU:HB3 | 7 | 0.18 | 0.07 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HA | 7 | 0.16 | 0.05 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HA | 7 | 0.16 | 0.05 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HA | 7 | 0.16 | 0.05 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD21 | 1:B:120:ILE:HA | 7 | 0.16 | 0.05 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2539) | 1:B:99:LEU:HD22 | 1:B:120:ILE:HA | 7 | 0.16 | 0.05 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD23 | 1:B:120:ILE:HA | 7 | 0.16 | 0.05 | 0.15 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD11 | 7 | 0.16 | 0.03 | 0.16 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD12 | 7 | 0.16 | 0.03 | 0.16 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD13 | 7 | 0.16 | 0.03 | 0.16 |
| (1,3936) | 1:B:134:ILE:H | 1:B:127:ARG:HG2 | 7 | 0.16 | 0.04 | 0.15 |
| (1,680) | 1:A:123:LYS:HA | 1:A:123:LYS:HG3 | 7 | 0.15 | 0.02 | 0.16 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD11 | 7 | 0.15 | 0.04 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD12 | 7 | 0.15 | 0.04 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD13 | 7 | 0.15 | 0.04 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD21 | 7 | 0.15 | 0.04 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD22 | 7 | 0.15 | 0.04 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD23 | 7 | 0.15 | 0.04 | 0.14 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG21 | 7 | 0.15 | 0.04 | 0.16 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG22 | 7 | 0.15 | 0.04 | 0.16 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG23 | 7 | 0.15 | 0.04 | 0.16 |
| (1,23) | 1:A:94:ARG:HA | 1:A:94:ARG:HB3 | 7 | 0.15 | 0.03 | 0.13 |
| (1,502) | 1:A:113:THR:HG21 | 1:A:150:PRO:HB3 | 7 | 0.14 | 0.04 | 0.12 |
| (1,502) | 1:A:113:THR:HG22 | 1:A:150:PRO:HB3 | 7 | 0.14 | 0.04 | 0.12 |
| (1,502) | 1:A:113:THR:HG23 | 1:A:150:PRO:HB3 | 7 | 0.14 | 0.04 | 0.12 |
| (1,1157) | 1:A:157:LEU:HB3 | 1:A:157:LEU:HG | 7 | 0.13 | 0.01 | 0.13 |
| (1,3288) | 1:B:148:VAL:HG11 | 1:B:153:VAL:HA | 7 | 0.13 | 0.03 | 0.12 |
| (1,3288) | 1:B:148:VAL:HG12 | 1:B:153:VAL:HA | 7 | 0.13 | 0.03 | 0.12 |
| (1,3288) | 1:B:148:VAL:HG13 | 1:B:153:VAL:HA | 7 | 0.13 | 0.03 | 0.12 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG21 | 6 | 1.4 | 0.99 | 1.37 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG22 | 6 | 1.4 | 0.99 | 1.37 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG23 | 6 | 1.4 | 0.99 | 1.37 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD2 | 6 | 1.36 | 0.48 | 1.54 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD3 | 6 | 1.36 | 0.48 | 1.54 |
| (1,1) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HA | 6 | 1.22 | 0.81 | 0.8 |
| (1,1) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HA | 6 | 1.22 | 0.81 | 0.8 |
| (1,1) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HA | 6 | 1.22 | 0.81 | 0.8 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD1 | 6 | 1.18 | 0.49 | 1.25 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD2 | 6 | 1.18 | 0.49 | 1.25 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD1 | 6 | 1.01 | 0.4 | 0.92 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD2 | 6 | 1.01 | 0.4 | 0.92 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG21 | 6 | 0.98 | 0.57 | 0.84 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG22 | 6 | 0.98 | 0.57 | 0.84 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG23 | 6 | 0.98 | 0.57 | 0.84 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE1 | 6 | 0.97 | 0.08 | 0.98 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE2 | 6 | 0.97 | 0.08 | 0.98 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE1 | 6 | 0.97 | 0.08 | 0.98 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE2 | 6 | 0.97 | 0.08 | 0.98 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE1 | 6 | 0.97 | 0.08 | 0.98 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE2 | 6 | 0.97 | 0.08 | 0.98 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE1 | 6 | 0.97 | 0.26 | 0.96 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE2 | 6 | 0.97 | 0.26 | 0.96 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB1 | 6 | 0.95 | 0.66 | 0.72 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB2 | 6 | 0.95 | 0.66 | 0.72 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB3 | 6 | 0.95 | 0.66 | 0.72 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD22 | 6 | 0.92 | 0.37 | 0.88 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD21 | 6 | 0.92 | 0.37 | 0.88 |
| (1,2025) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 6 | 0.84 | 0.48 | 0.89 |
| (1,2157) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 6 | 0.84 | 0.48 | 0.89 |
| (1,2284) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB2 | 6 | 0.8 | 0.5 | 0.74 |
| (1,2284) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB2 | 6 | 0.8 | 0.5 | 0.74 |
| (1,990) | 1:A:148:VAL:HA | 1:A:169:MET:HB2 | 6 | 0.75 | 0.32 | 0.85 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE1 | 6 | 0.72 | 0.34 | 0.83 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE2 | 6 | 0.72 | 0.34 | 0.83 |
| (1,1012) | 1:A:148:VAL:HG11 | 1:A:169:MET:HB2 | 6 | 0.68 | 0.28 | 0.78 |
| (1,1012) | 1:A:148:VAL:HG12 | 1:A:169:MET:HB2 | 6 | 0.68 | 0.28 | 0.78 |
| (1,1012) | 1:A:148:VAL:HG13 | 1:A:169:MET:HB2 | 6 | 0.68 | 0.28 | 0.78 |
| (1,710) | 1:A:126:GLU:HA | 1:A:135:SER:HB2 | 6 | 0.65 | 0.28 | 0.66 |
| (1,1916) | 1:A:162:THR:H | 1:A:102:ASN:HB3 | 6 | 0.63 | 0.21 | 0.58 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG21 | 6 | 0.63 | 0.08 | 0.64 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG22 | 6 | 0.63 | 0.08 | 0.64 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG23 | 6 | 0.63 | 0.08 | 0.64 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD11 | 6 | 0.62 | 0.22 | 0.63 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD12 | 6 | 0.62 | 0.22 | 0.63 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD13 | 6 | 0.62 | 0.22 | 0.63 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD21 | 6 | 0.62 | 0.22 | 0.63 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD22 | 6 | 0.62 | 0.22 | 0.63 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD23 | 6 | 0.62 | 0.22 | 0.63 |
| (1,722) | 1:A:126:GLU:HG2 | 1:A:135:SER:HA | 6 | 0.6 | 0.25 | 0.48 |
| (1,2716) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG13 | 6 | 0.58 | 0.05 | 0.6 |
| (1,2716) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG13 | 6 | 0.58 | 0.05 | 0.6 |
| (1,2716) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG13 | 6 | 0.58 | 0.05 | 0.6 |
| (1,2716) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG13 | 6 | 0.58 | 0.05 | 0.6 |
| (1,2716) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG13 | 6 | 0.58 | 0.05 | 0.6 |
| (1,2716) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG13 | 6 | 0.58 | 0.05 | 0.6 |
| (1,2907) | 1:B:120:ILE:HA | 1:B:120:ILE:HG13 | 6 | 0.55 | 0.03 | 0.54 |
| (1,688) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB3 | 6 | 0.52 | 0.18 | 0.5 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB1 | 6 | 0.49 | 0.26 | 0.6 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB2 | 6 | 0.49 | 0.26 | 0.6 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB3 | 6 | 0.49 | 0.26 | 0.6 |
| (1,684) | 1:A:123:LYS:HA | 1:A:135:SER:HB3 | 6 | 0.48 | 0.3 | 0.49 |
| (1,1998) | 1:A:169:MET:H | 1:A:169:MET:HB2 | 6 | 0.46 | 0.26 | 0.34 |
| (1,723) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB2 | 6 | 0.44 | 0.16 | 0.5 |
| (1,3612) | 1:B:95:TRP:H | 1:B:95:TRP:HB2 | 6 | 0.44 | 0.05 | 0.43 |
| (1,827) | 1:A:139:THR:HA | 1:A:140:ARG:HG2 | 6 | 0.43 | 0.26 | 0.28 |
| (1,99) | 1:A:96:ARG:HB3 | 1:A:164:THR:HB | 6 | 0.43 | 0.16 | 0.37 |
| (1,2081) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 6 | 0.43 | 0.22 | 0.38 |
| (1,2213) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 6 | 0.43 | 0.22 | 0.38 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB1 | 6 | 0.39 | 0.2 | 0.47 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB2 | 6 | 0.39 | 0.2 | 0.47 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB3 | 6 | 0.39 | 0.2 | 0.47 |
| (1,3460) | 1:B:157:LEU:HD21 | 1:B:163:LEU:HB3 | 6 | 0.38 | 0.11 | 0.42 |
| (1,3460) | 1:B:157:LEU:HD22 | 1:B:163:LEU:HB3 | 6 | 0.38 | 0.11 | 0.42 |
| (1,3460) | 1:B:157:LEU:HD23 | 1:B:163:LEU:HB3 | 6 | 0.38 | 0.11 | 0.42 |
| (1,3491) | 1:B:160:GLU:HB2 | 1:B:162:THR:HB | 6 | 0.38 | 0.12 | 0.38 |
| (1,3137) | 1:B:141:LYS:HG2 | 1:B:142:TYR:HB3 | 6 | 0.38 | 0.11 | 0.37 |
| (1,4197) | 1:B:162:THR:H | 1:B:102:ASN:HB3 | 6 | 0.38 | 0.22 | 0.37 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD3 | 6 | 0.35 | 0.11 | 0.35 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD2 | 6 | 0.35 | 0.11 | 0.35 |
| (1,2037) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 6 | 0.35 | 0.11 | 0.34 |
| (1,2169) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 6 | 0.35 | 0.11 | 0.34 |
| (1,9) | 1:A:90:HIS:HB3 | 1:A:91:THR:HA | 6 | 0.33 | 0.18 | 0.27 |
| (1,3847) | 1:B:123:LYS:H | 1:B:109:LEU:HB2 | 6 | 0.32 | 0.06 | 0.32 |
| (1,1210) | 1:A:160:GLU:HB2 | 1:A:162:THR:HB | 6 | 0.3 | 0.14 | 0.23 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG21 | 6 | 0.29 | 0.02 | 0.3 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG22 | 6 | 0.29 | 0.02 | 0.3 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG23 | 6 | 0.29 | 0.02 | 0.3 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD11 | 6 | 0.29 | 0.03 | 0.3 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD12 | 6 | 0.29 | 0.03 | 0.3 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD13 | 6 | 0.29 | 0.03 | 0.3 |
| (1,3748) | 1:B:113:THR:H | 1:B:112:LYS:HB2 | 6 | 0.29 | 0.08 | 0.28 |
| (1,3139) | 1:B:141:LYS:HG3 | 1:B:141:LYS:HE2 | 6 | 0.29 | 0.05 | 0.3 |
| (1,4262) | 1:B:167:ALA:H | 1:B:166:GLU:HB2 | 6 | 0.28 | 0.14 | 0.26 |
| (1,3436) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HA | 6 | 0.26 | 0.13 | 0.24 |
| (1,1634) | 1:A:131:HIS:H | 1:A:129:ASP:HB3 | 6 | 0.24 | 0.06 | 0.22 |
| (1,3018) | 1:B:127:ARG:HA | 1:B:127:ARG:HD3 | 6 | 0.24 | 0.07 | 0.25 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG2 | 6 | 0.23 | 0.07 | 0.25 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG3 | 6 | 0.23 | 0.07 | 0.25 |
| (1,2738) | 1:B:112:LYS:HB2 | 1:B:120:ILE:HA | 6 | 0.23 | 0.08 | 0.22 |
| (1,4128) | 1:B:155:SER:H | 1:B:154:SER:HB2 | 6 | 0.22 | 0.08 | 0.22 |
| (1,2929) | 1:B:120:ILE:HG21 | 1:B:139:THR:HA | 6 | 0.22 | 0.06 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2929) | 1:B:120:ILE:HG22 | 1:B:139:THR:HA | 6 | 0.22 | 0.06 | 0.22 |
| (1,2929) | 1:B:120:ILE:HG23 | 1:B:139:THR:HA | 6 | 0.22 | 0.06 | 0.22 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD1 | 6 | 0.21 | 0.07 | 0.22 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD2 | 6 | 0.21 | 0.07 | 0.22 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD1 | 6 | 0.21 | 0.07 | 0.22 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD2 | 6 | 0.21 | 0.07 | 0.22 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD1 | 6 | 0.21 | 0.07 | 0.22 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD2 | 6 | 0.21 | 0.07 | 0.22 |
| (1,1173) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB3 | 6 | 0.2 | 0.04 | 0.2 |
| (1,1173) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB3 | 6 | 0.2 | 0.04 | 0.2 |
| (1,1173) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB3 | 6 | 0.2 | 0.04 | 0.2 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD21 | 6 | 0.19 | 0.06 | 0.2 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD22 | 6 | 0.19 | 0.06 | 0.2 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD23 | 6 | 0.19 | 0.06 | 0.2 |
| (1,2928) | 1:B:120:ILE:HG21 | 1:B:122:GLY:HA3 | 6 | 0.19 | 0.05 | 0.18 |
| (1,2928) | 1:B:120:ILE:HG22 | 1:B:122:GLY:HA3 | 6 | 0.19 | 0.05 | 0.18 |
| (1,2928) | 1:B:120:ILE:HG23 | 1:B:122:GLY:HA3 | 6 | 0.19 | 0.05 | 0.18 |
| (1,1258) | 1:A:166:GLU:HG2 | 1:A:167:ALA:HA | 6 | 0.19 | 0.06 | 0.18 |
| (1,1258) | 1:A:166:GLU:HG3 | 1:A:167:ALA:HA | 6 | 0.19 | 0.06 | 0.18 |
| (1,279) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA2 | 6 | 0.18 | 0.03 | 0.18 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,3358) | 1:B:153:VAL:HA | 1:B:168:PRO:HD2 | 6 | 0.18 | 0.03 | 0.18 |
| (1,652) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HB2 | 6 | 0.17 | 0.09 | 0.14 |
| (1,652) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HB2 | 6 | 0.17 | 0.09 | 0.14 |
| (1,652) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HB2 | 6 | 0.17 | 0.09 | 0.14 |
| (1,1647) | 1:A:132:GLY:H | 1:A:131:HIS:HB3 | 6 | 0.17 | 0.03 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG21 | 6 | 0.17 | 0.03 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG22 | 6 | 0.17 | 0.03 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG23 | 6 | 0.17 | 0.03 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG11 | 6 | 0.17 | 0.03 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG12 | 6 | 0.17 | 0.03 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG13 | 6 | 0.17 | 0.03 | 0.18 |
| (1,4263) | 1:B:167:ALA:H | 1:B:166:GLU:HB3 | 6 | 0.17 | 0.06 | 0.16 |
| (1,664) | 1:A:121:THR:HA | 1:A:139:THR:HA | 6 | 0.17 | 0.04 | 0.16 |
| (1,1391) | 1:A:105:ALA:H | 1:A:108:GLU:HB3 | 6 | 0.16 | 0.03 | 0.18 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD11 | 6 | 0.15 | 0.02 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD12 | 6 | 0.15 | 0.02 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD13 | 6 | 0.15 | 0.02 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD21 | 6 | 0.15 | 0.02 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD22 | 6 | 0.15 | 0.02 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD23 | 6 | 0.15 | 0.02 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,465) | 1:A:112:LYS:HG2 | 1:A:118:VAL:HA | 6 | 0.15 | 0.03 | 0.14 |
| (1,465) | 1:A:112:LYS:HG3 | 1:A:118:VAL:HA | 6 | 0.15 | 0.03 | 0.14 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG3 | 6 | 0.15 | 0.03 | 0.15 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG2 | 6 | 0.15 | 0.03 | 0.15 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD1 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD2 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD1 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD2 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD1 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD2 | 6 | 0.14 | 0.04 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD21 | 6 | 0.14 | 0.02 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD22 | 6 | 0.14 | 0.02 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD23 | 6 | 0.14 | 0.02 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD21 | 6 | 0.14 | 0.02 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD22 | 6 | 0.14 | 0.02 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD23 | 6 | 0.14 | 0.02 | 0.14 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 6 | 0.14 | 0.02 | 0.15 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 6 | 0.14 | 0.02 | 0.15 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 6 | 0.14 | 0.02 | 0.15 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 6 | 0.14 | 0.02 | 0.15 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 6 | 0.14 | 0.02 | 0.15 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 6 | 0.14 | 0.02 | 0.15 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 6 | 0.14 | 0.02 | 0.15 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 6 | 0.14 | 0.02 | 0.15 |
| (1,3592) | 1:B:170:PRO:HB2 | 1:B:170:PRO:HG2 | 6 | 0.11 | 0.0 | 0.11 |
| (1,2004) | 1:A:171:LYS:H | 1:A:169:MET:HA | 5 | 1.01 | 0.29 | 0.87 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD11 | 5 | 0.97 | 0.27 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD12 | 5 | 0.97 | 0.27 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD13 | 5 | 0.97 | 0.27 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD21 | 5 | 0.97 | 0.27 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD22 | 5 | 0.97 | 0.27 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD23 | 5 | 0.97 | 0.27 | 1.13 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG2 | 5 | 0.84 | 0.46 | 0.78 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG3 | 5 | 0.84 | 0.46 | 0.78 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG3 | 5 | 0.78 | 0.24 | 0.76 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG2 | 5 | 0.78 | 0.24 | 0.76 |
| (1,3346) | 1:B:152:GLN:HB2 | 1:B:169:MET:HA | 5 | 0.71 | 0.27 | 0.77 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD2 | 5 | 0.67 | 0.12 | 0.69 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD3 | 5 | 0.67 | 0.12 | 0.69 |
| (1,7) | 1:A:90:HIS:HB2 | 1:A:91:THR:HA | 5 | 0.65 | 0.26 | 0.63 |
| (1,1691) | 1:A:140:ARG:H | 1:A:120:ILE:HB | 5 | 0.64 | 0.09 | 0.65 |
| (1,2062) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 5 | 0.63 | 0.34 | 0.49 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2194) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 5 | 0.63 | 0.34 | 0.49 |
| (1,4255) | 1:B:167:ALA:H | 1:B:95:TRP:HB3 | 5 | 0.63 | 0.22 | 0.63 |
| (1,3763) | 1:B:114:LYS:H | 1:B:115:ASP:HB2 | 5 | 0.61 | 0.23 | 0.64 |
| (1,626) | 1:A:120:ILE:HA | 1:A:120:ILE:HG13 | 5 | 0.56 | 0.02 | 0.55 |
| (1,232) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HG12 | 5 | 0.52 | 0.16 | 0.59 |
| (1,232) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HG12 | 5 | 0.52 | 0.16 | 0.59 |
| (1,232) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HG12 | 5 | 0.52 | 0.16 | 0.59 |
| (1,2314) | 1:B:94:ARG:HA | 1:B:169:MET:HB2 | 5 | 0.51 | 0.12 | 0.45 |
| (1,3005) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB3 | 5 | 0.5 | 0.47 | 0.22 |
| (1,3274) | 1:B:148:VAL:HA | 1:B:170:PRO:HG2 | 5 | 0.46 | 0.27 | 0.48 |
| (1,1799) | 1:A:152:GLN:HE21 | 1:A:152:GLN:HB3 | 5 | 0.45 | 0.2 | 0.43 |
| (1,2325) | 1:B:94:ARG:HG2 | 1:B:166:GLU:HB2 | 5 | 0.45 | 0.18 | 0.48 |
| (1,2325) | 1:B:94:ARG:HG3 | 1:B:166:GLU:HB2 | 5 | 0.45 | 0.18 | 0.48 |
| (1,4280) | 1:B:169:MET:H | 1:B:169:MET:HB3 | 5 | 0.45 | 0.23 | 0.45 |
| (1,435) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG13 | 5 | 0.41 | 0.1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG13 | 5 | 0.41 | 0.1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG13 | 5 | 0.41 | 0.1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG13 | 5 | 0.41 | 0.1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG13 | 5 | 0.41 | 0.1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG13 | 5 | 0.41 | 0.1 | 0.41 |
| (1,2000) | 1:A:169:MET:H | 1:A:169:MET:HG3 | 5 | 0.4 | 0.23 | 0.5 |
| (1,3345) | 1:B:152:GLN:HB2 | 1:B:168:PRO:HD3 | 5 | 0.4 | 0.23 | 0.38 |
| (1,528) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HB | 5 | 0.36 | 0.08 | 0.33 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD1 | 5 | 0.33 | 0.04 | 0.33 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD2 | 5 | 0.33 | 0.04 | 0.33 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD1 | 5 | 0.33 | 0.04 | 0.33 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD2 | 5 | 0.33 | 0.04 | 0.33 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD1 | 5 | 0.33 | 0.04 | 0.33 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD2 | 5 | 0.33 | 0.04 | 0.33 |
| (1,3902) | 1:B:129:ASP:H | 1:B:129:ASP:HB2 | 5 | 0.32 | 0.06 | 0.34 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD11 | 5 | 0.32 | 0.12 | 0.26 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD12 | 5 | 0.32 | 0.12 | 0.26 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD13 | 5 | 0.32 | 0.12 | 0.26 |
| (1,4205) | 1:B:162:THR:H | 1:B:160:GLU:HB2 | 5 | 0.31 | 0.08 | 0.31 |
| (1,3409) | 1:B:155:SER:HB3 | 1:B:157:LEU:HB3 | 5 | 0.3 | 0.07 | 0.3 |
| (1,3409) | 1:B:155:SER:HB2 | 1:B:157:LEU:HB3 | 5 | 0.3 | 0.07 | 0.3 |
| (1,3848) | 1:B:123:LYS:H | 1:B:109:LEU:HG | 5 | 0.3 | 0.13 | 0.24 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE1 | 5 | 0.29 | 0.1 | 0.28 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE2 | 5 | 0.29 | 0.1 | 0.28 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG21 | 5 | 0.27 | 0.03 | 0.27 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG22 | 5 | 0.27 | 0.03 | 0.27 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG23 | 5 | 0.27 | 0.03 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1847) | 1:A:155:SER:H | 1:A:154:SER:HB2 | 5 | 0.27 | 0.07 | 0.29 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD11 | 5 | 0.27 | 0.15 | 0.21 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD12 | 5 | 0.27 | 0.15 | 0.21 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD13 | 5 | 0.27 | 0.15 | 0.21 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD11 | 5 | 0.25 | 0.07 | 0.27 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD12 | 5 | 0.25 | 0.07 | 0.27 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD13 | 5 | 0.25 | 0.07 | 0.27 |
| (1,3915) | 1:B:131:HIS:H | 1:B:129:ASP:HB3 | 5 | 0.25 | 0.08 | 0.26 |
| (1,1816) | 1:A:153:VAL:H | 1:A:149:ASP:HB2 | 5 | 0.24 | 0.11 | 0.21 |
| (1,1065) | 1:A:152:GLN:HB2 | 1:A:169:MET:HA | 5 | 0.24 | 0.07 | 0.24 |
| (1,858) | 1:A:141:LYS:HG3 | 1:A:141:LYS:HE2 | 5 | 0.22 | 0.07 | 0.2 |
| (1,1626) | 1:A:129:ASP:H | 1:A:132:GLY:HA3 | 5 | 0.22 | 0.04 | 0.23 |
| (1,3249) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA3 | 5 | 0.22 | 0.18 | 0.13 |
| (1,3474) | 1:B:158:SER:HB3 | 1:B:160:GLU:HB3 | 5 | 0.22 | 0.12 | 0.13 |
| (1,3955) | 1:B:137:CYS:H | 1:B:136:ARG:HB3 | 5 | 0.21 | 0.07 | 0.22 |
| (1,4182) | 1:B:161:GLY:H | 1:B:102:ASN:HB2 | 5 | 0.2 | 0.08 | 0.2 |
| (1,654) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HD2 | 5 | 0.2 | 0.08 | 0.16 |
| (1,654) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HD2 | 5 | 0.2 | 0.08 | 0.16 |
| (1,654) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HD2 | 5 | 0.2 | 0.08 | 0.16 |
| (1,1598) | 1:A:128:GLN:H | 1:A:127:ARG:HG2 | 5 | 0.2 | 0.08 | 0.22 |
| (1,3454) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB3 | 5 | 0.19 | 0.05 | 0.17 |
| (1,3454) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB3 | 5 | 0.19 | 0.05 | 0.17 |
| (1,3454) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB3 | 5 | 0.19 | 0.05 | 0.17 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD11 | 5 | 0.18 | 0.05 | 0.18 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD12 | 5 | 0.18 | 0.05 | 0.18 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD13 | 5 | 0.18 | 0.05 | 0.18 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB2 | 5 | 0.18 | 0.05 | 0.17 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB3 | 5 | 0.18 | 0.05 | 0.17 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG3 | 5 | 0.18 | 0.07 | 0.15 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG2 | 5 | 0.18 | 0.07 | 0.15 |
| (1,1525) | 1:A:119:GLU:H | 1:A:114:LYS:HB3 | 5 | 0.17 | 0.05 | 0.17 |
| (1,3430) | 1:B:157:LEU:HA | 1:B:163:LEU:HB3 | 5 | 0.17 | 0.02 | 0.16 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD2 | 5 | 0.17 | 0.06 | 0.15 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD2 | 5 | 0.17 | 0.06 | 0.15 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD3 | 5 | 0.17 | 0.06 | 0.15 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD3 | 5 | 0.17 | 0.06 | 0.15 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD2 | 5 | 0.17 | 0.04 | 0.17 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD3 | 5 | 0.17 | 0.04 | 0.17 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB2 | 5 | 0.16 | 0.03 | 0.16 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB3 | 5 | 0.16 | 0.03 | 0.16 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG21 | 5 | 0.16 | 0.04 | 0.14 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG22 | 5 | 0.16 | 0.04 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG23 | 5 | 0.16 | 0.04 | 0.14 |
| (1,258) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HA | 5 | 0.16 | 0.07 | 0.14 |
| (1,258) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HA | 5 | 0.16 | 0.07 | 0.14 |
| (1,258) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HA | 5 | 0.16 | 0.07 | 0.14 |
| (1,258) | 1:A:99:LEU:HD21 | 1:A:120:ILE:HA | 5 | 0.16 | 0.07 | 0.14 |
| (1,258) | 1:A:99:LEU:HD22 | 1:A:120:ILE:HA | 5 | 0.16 | 0.07 | 0.14 |
| (1,258) | 1:A:99:LEU:HD23 | 1:A:120:ILE:HA | 5 | 0.16 | 0.07 | 0.14 |
| (1,1901) | 1:A:161:GLY:H | 1:A:102:ASN:HB2 | 5 | 0.16 | 0.02 | 0.16 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG21 | 5 | 0.16 | 0.03 | 0.15 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG22 | 5 | 0.16 | 0.03 | 0.15 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG23 | 5 | 0.16 | 0.03 | 0.15 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD11 | 5 | 0.16 | 0.06 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD12 | 5 | 0.16 | 0.06 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD13 | 5 | 0.16 | 0.06 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD21 | 5 | 0.16 | 0.06 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD22 | 5 | 0.16 | 0.06 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD23 | 5 | 0.16 | 0.06 | 0.13 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB2 | 5 | 0.16 | 0.04 | 0.16 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB3 | 5 | 0.16 | 0.04 | 0.16 |
| (1,605) | 1:A:119:GLU:HA | 1:A:120:ILE:HG13 | 5 | 0.15 | 0.01 | 0.16 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD21 | 5 | 0.15 | 0.03 | 0.16 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD22 | 5 | 0.15 | 0.03 | 0.16 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD23 | 5 | 0.15 | 0.03 | 0.16 |
| (1,1282) | 1:A:168:PRO:HB3 | 1:A:169:MET:HA | 5 | 0.15 | 0.04 | 0.14 |
| (1,3391) | 1:B:155:SER:HA | 1:B:165:VAL:HA | 5 | 0.15 | 0.03 | 0.15 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG21 | 5 | 0.14 | 0.02 | 0.15 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG22 | 5 | 0.14 | 0.02 | 0.15 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG23 | 5 | 0.14 | 0.02 | 0.15 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE1 | 5 | 0.14 | 0.04 | 0.13 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE2 | 5 | 0.14 | 0.04 | 0.13 |
| (1,1588) | 1:A:126:GLU:H | 1:A:125:GLU:HG3 | 5 | 0.14 | 0.02 | 0.13 |
| (1,4034) | 1:B:148:VAL:H | 1:B:149:ASP:H | 5 | 0.14 | 0.04 | 0.13 |
| (1,2442) | 1:B:97:VAL:HG21 | 1:B:166:GLU:HA | 5 | 0.14 | 0.03 | 0.12 |
| (1,2442) | 1:B:97:VAL:HG22 | 1:B:166:GLU:HA | 5 | 0.14 | 0.03 | 0.12 |
| (1,2442) | 1:B:97:VAL:HG23 | 1:B:166:GLU:HA | 5 | 0.14 | 0.03 | 0.12 |
| (1,1110) | 1:A:155:SER:HA | 1:A:165:VAL:HA | 5 | 0.14 | 0.01 | 0.14 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG21 | 5 | 0.14 | 0.03 | 0.13 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG22 | 5 | 0.14 | 0.03 | 0.13 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG23 | 5 | 0.14 | 0.03 | 0.13 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG11 | 5 | 0.14 | 0.01 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG12 | 5 | 0.14 | 0.01 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG13 | 5 | 0.14 | 0.01 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG21 | 5 | 0.14 | 0.01 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG22 | 5 | 0.14 | 0.01 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG23 | 5 | 0.14 | 0.01 | 0.14 |
| (1,1079) | 1:A:153:VAL:HB | 1:A:154:SER:HA | 5 | 0.13 | 0.01 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG11 | 5 | 0.13 | 0.02 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG12 | 5 | 0.13 | 0.02 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG13 | 5 | 0.13 | 0.02 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG21 | 5 | 0.13 | 0.02 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG22 | 5 | 0.13 | 0.02 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG23 | 5 | 0.13 | 0.02 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD11 | 5 | 0.13 | 0.01 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD12 | 5 | 0.13 | 0.01 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD13 | 5 | 0.13 | 0.01 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD21 | 5 | 0.13 | 0.01 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD22 | 5 | 0.13 | 0.01 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD23 | 5 | 0.13 | 0.01 | 0.13 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG11 | 5 | 0.12 | 0.01 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG12 | 5 | 0.12 | 0.01 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG13 | 5 | 0.12 | 0.01 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG21 | 5 | 0.12 | 0.01 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG22 | 5 | 0.12 | 0.01 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG23 | 5 | 0.12 | 0.01 | 0.12 |
| (1,734) | 1:A:127:ARG:HA | 1:A:127:ARG:HB3 | 5 | 0.12 | 0.02 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD11 | 5 | 0.12 | 0.01 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD12 | 5 | 0.12 | 0.01 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD13 | 5 | 0.12 | 0.01 | 0.11 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD1 | 5 | 0.12 | 0.01 | 0.11 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD2 | 5 | 0.12 | 0.01 | 0.11 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD1 | 5 | 0.12 | 0.01 | 0.11 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD2 | 5 | 0.12 | 0.01 | 0.11 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD1 | 5 | 0.12 | 0.01 | 0.11 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD2 | 5 | 0.12 | 0.01 | 0.11 |
| (1,1311) | 1:A:170:PRO:HB2 | 1:A:170:PRO:HG2 | 5 | 0.12 | 0.01 | 0.11 |
| (1,724) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB3 | 4 | 0.95 | 0.32 | 1.06 |
| (1,16) | 1:A:93:ASP:HA | 1:A:94:ARG:HD2 | 4 | 0.86 | 0.4 | 0.8 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD22 | 4 | 0.84 | 0.38 | 0.94 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD21 | 4 | 0.84 | 0.38 | 0.94 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB2 | 4 | 0.83 | 0.49 | 0.92 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB3 | 4 | 0.83 | 0.49 | 0.92 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD2 | 4 | 0.78 | 0.67 | 0.45 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD3 | 4 | 0.78 | 0.67 | 0.45 |
| (1,728) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HA | 4 | 0.62 | 0.21 | 0.64 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3895) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB2 | 4 | 0.55 | 0.14 | 0.5 |
| (1,1288) | 1:A:169:MET:HA | 1:A:169:MET:HG2 | 4 | 0.52 | 0.11 | 0.52 |
| (1,44) | 1:A:94:ARG:HG2 | 1:A:166:GLU:HB2 | 4 | 0.51 | 0.38 | 0.36 |
| (1,44) | 1:A:94:ARG:HG3 | 1:A:166:GLU:HB2 | 4 | 0.51 | 0.38 | 0.36 |
| (1,4024) | 1:B:148:VAL:H | 1:B:146:PRO:HB3 | 4 | 0.5 | 0.1 | 0.53 |
| (1,1322) | 1:A:94:ARG:H | 1:A:93:ASP:HB2 | 4 | 0.48 | 0.11 | 0.48 |
| (1,2318) | 1:B:94:ARG:HB2 | 1:B:96:ARG:HA | 4 | 0.47 | 0.33 | 0.36 |
| (1,3972) | 1:B:140:ARG:H | 1:B:120:ILE:HB | 4 | 0.47 | 0.12 | 0.5 |
| (1,3116) | 1:B:139:THR:HG21 | 1:B:141:LYS:HE2 | 4 | 0.45 | 0.14 | 0.49 |
| (1,3116) | 1:B:139:THR:HG22 | 1:B:141:LYS:HE2 | 4 | 0.45 | 0.14 | 0.49 |
| (1,3116) | 1:B:139:THR:HG23 | 1:B:141:LYS:HE2 | 4 | 0.45 | 0.14 | 0.49 |
| (1,1114) | 1:A:155:SER:HB2 | 1:A:163:LEU:HA | 4 | 0.45 | 0.16 | 0.48 |
| (1,2148) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 4 | 0.44 | 0.23 | 0.38 |
| (1,2281) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 4 | 0.44 | 0.23 | 0.38 |
| (1,2980) | 1:B:125:GLU:HA | 1:B:125:GLU:HG2 | 4 | 0.42 | 0.15 | 0.5 |
| (1,2299) | 1:B:93:ASP:HB2 | 1:B:94:ARG:HA | 4 | 0.4 | 0.08 | 0.37 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB2 | 4 | 0.4 | 0.21 | 0.4 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB3 | 4 | 0.4 | 0.21 | 0.4 |
| (1,3569) | 1:B:169:MET:HA | 1:B:169:MET:HG2 | 4 | 0.4 | 0.23 | 0.4 |
| (1,2930) | 1:B:120:ILE:HG21 | 1:B:140:ARG:HA | 4 | 0.38 | 0.14 | 0.36 |
| (1,2930) | 1:B:120:ILE:HG22 | 1:B:140:ARG:HA | 4 | 0.38 | 0.14 | 0.36 |
| (1,2930) | 1:B:120:ILE:HG23 | 1:B:140:ARG:HA | 4 | 0.38 | 0.14 | 0.36 |
| (1,1277) | 1:A:168:PRO:HA | 1:A:169:MET:HG3 | 4 | 0.38 | 0.24 | 0.38 |
| (1,4084) | 1:B:152:GLN:HE21 | 1:B:168:PRO:HD2 | 4 | 0.38 | 0.13 | 0.39 |
| (1,1756) | 1:A:148:VAL:H | 1:A:170:PRO:HG3 | 4 | 0.36 | 0.13 | 0.36 |
| (1,1664) | 1:A:135:SER:H | 1:A:134:ILE:HG13 | 4 | 0.36 | 0.11 | 0.38 |
| (1,2971) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HB2 | 4 | 0.35 | 0.12 | 0.34 |
| (1,1085) | 1:A:153:VAL:HG11 | 1:A:155:SER:HB3 | 4 | 0.34 | 0.19 | 0.29 |
| (1,1085) | 1:A:153:VAL:HG12 | 1:A:155:SER:HB3 | 4 | 0.34 | 0.19 | 0.29 |
| (1,1085) | 1:A:153:VAL:HG13 | 1:A:155:SER:HB3 | 4 | 0.34 | 0.19 | 0.29 |
| (1,1085) | 1:A:153:VAL:HG21 | 1:A:155:SER:HB3 | 4 | 0.34 | 0.19 | 0.29 |
| (1,1085) | 1:A:153:VAL:HG22 | 1:A:155:SER:HB3 | 4 | 0.34 | 0.19 | 0.29 |
| (1,1085) | 1:A:153:VAL:HG23 | 1:A:155:SER:HB3 | 4 | 0.34 | 0.19 | 0.29 |
| (1,690) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HB2 | 4 | 0.34 | 0.13 | 0.38 |
| (1,3604) | 1:B:94:ARG:H | 1:B:93:ASP:HB3 | 4 | 0.32 | 0.11 | 0.29 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD3 | 4 | 0.32 | 0.21 | 0.22 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD2 | 4 | 0.32 | 0.21 | 0.22 |
| (1,1642) | 1:A:132:GLY:H | 1:A:129:ASP:HB2 | 4 | 0.29 | 0.16 | 0.26 |
| (1,2332) | 1:B:95:TRP:HA | 1:B:95:TRP:HB2 | 4 | 0.27 | 0.08 | 0.25 |
| (1,2568) | 1:B:105:ALA:HA | 1:B:108:GLU:HB3 | 4 | 0.27 | 0.1 | 0.29 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG3 | 4 | 0.26 | 0.05 | 0.26 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG2 | 4 | 0.26 | 0.05 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2617) | 1:B:108:GLU:HA | 1:B:108:GLU:HG2 | 4 | 0.26 | 0.1 | 0.28 |
| (1,2935) | 1:B:120:ILE:HD11 | 1:B:140:ARG:HD2 | 4 | 0.26 | 0.1 | 0.26 |
| (1,2935) | 1:B:120:ILE:HD12 | 1:B:140:ARG:HD2 | 4 | 0.26 | 0.1 | 0.26 |
| (1,2935) | 1:B:120:ILE:HD13 | 1:B:140:ARG:HD2 | 4 | 0.26 | 0.1 | 0.26 |
| (1,3935) | 1:B:134:ILE:H | 1:B:127:ARG:HB2 | 4 | 0.26 | 0.08 | 0.29 |
| (1,3302) | 1:B:148:VAL:HG21 | 1:B:169:MET:HB3 | 4 | 0.25 | 0.06 | 0.25 |
| (1,3302) | 1:B:148:VAL:HG22 | 1:B:169:MET:HB3 | 4 | 0.25 | 0.06 | 0.25 |
| (1,3302) | 1:B:148:VAL:HG23 | 1:B:169:MET:HB3 | 4 | 0.25 | 0.06 | 0.25 |
| (1,457) | 1:A:112:LYS:HB2 | 1:A:120:ILE:HA | 4 | 0.24 | 0.06 | 0.22 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD1 | 4 | 0.24 | 0.12 | 0.2 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD2 | 4 | 0.24 | 0.12 | 0.2 |
| (1,3910) | 1:B:129:ASP:H | 1:B:133:TYR:HB2 | 4 | 0.24 | 0.1 | 0.2 |
| (1,3806) | 1:B:119:GLU:H | 1:B:114:LYS:HB3 | 4 | 0.23 | 0.1 | 0.2 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD1 | 4 | 0.23 | 0.1 | 0.23 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD2 | 4 | 0.23 | 0.1 | 0.23 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD1 | 4 | 0.23 | 0.1 | 0.23 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD2 | 4 | 0.23 | 0.1 | 0.23 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD1 | 4 | 0.23 | 0.1 | 0.23 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD2 | 4 | 0.23 | 0.1 | 0.23 |
| (1,3907) | 1:B:129:ASP:H | 1:B:132:GLY:HA3 | 4 | 0.23 | 0.07 | 0.21 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG21 | 4 | 0.22 | 0.1 | 0.2 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG22 | 4 | 0.22 | 0.1 | 0.2 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG23 | 4 | 0.22 | 0.1 | 0.2 |
| (1,1743) | 1:A:148:VAL:H | 1:A:146:PRO:HB3 | 4 | 0.22 | 0.15 | 0.15 |
| (1,3138) | 1:B:141:LYS:HG2 | 1:B:143:THR:HA | 4 | 0.22 | 0.04 | 0.22 |
| (1,1902) | 1:A:161:GLY:H | 1:A:102:ASN:HB3 | 4 | 0.21 | 0.06 | 0.2 |
| (1,831) | 1:A:139:THR:HB | 1:A:141:LYS:HE2 | 4 | 0.21 | 0.06 | 0.21 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD11 | 4 | 0.21 | 0.05 | 0.23 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD12 | 4 | 0.21 | 0.05 | 0.23 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD13 | 4 | 0.21 | 0.05 | 0.23 |
| (1,1580) | 1:A:125:GLU:H | 1:A:108:GLU:HG2 | 4 | 0.2 | 0.06 | 0.22 |
| (1,648) | 1:A:120:ILE:HG21 | 1:A:139:THR:HA | 4 | 0.2 | 0.08 | 0.2 |
| (1,648) | 1:A:120:ILE:HG22 | 1:A:139:THR:HA | 4 | 0.2 | 0.08 | 0.2 |
| (1,648) | 1:A:120:ILE:HG23 | 1:A:139:THR:HA | 4 | 0.2 | 0.08 | 0.2 |
| (1,1796) | 1:A:152:GLN:HE21 | 1:A:149:ASP:HB2 | 4 | 0.2 | 0.04 | 0.22 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD1 | 4 | 0.2 | 0.06 | 0.22 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD2 | 4 | 0.2 | 0.06 | 0.22 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD3 | 4 | 0.2 | 0.04 | 0.2 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD2 | 4 | 0.2 | 0.04 | 0.2 |
| (1,337) | 1:A:108:GLU:HA | 1:A:108:GLU:HG3 | 4 | 0.2 | 0.04 | 0.18 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD3 | 4 | 0.2 | 0.06 | 0.18 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD2 | 4 | 0.2 | 0.06 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2560) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA2 | 4 | 0.19 | 0.03 | 0.2 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB2 | 4 | 0.19 | 0.02 | 0.19 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB3 | 4 | 0.19 | 0.02 | 0.19 |
| (1,2945) | 1:B:121:THR:HA | 1:B:139:THR:HA | 4 | 0.19 | 0.03 | 0.19 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG11 | 4 | 0.18 | 0.07 | 0.17 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG12 | 4 | 0.18 | 0.07 | 0.17 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG13 | 4 | 0.18 | 0.07 | 0.17 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG11 | 4 | 0.18 | 0.07 | 0.17 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG12 | 4 | 0.18 | 0.07 | 0.17 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG13 | 4 | 0.18 | 0.07 | 0.17 |
| (1,782) | 1:A:131:HIS:HB2 | 1:A:132:GLY:HA2 | 4 | 0.18 | 0.06 | 0.16 |
| (1,1655) | 1:A:134:ILE:H | 1:A:127:ARG:HG2 | 4 | 0.18 | 0.04 | 0.18 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG21 | 4 | 0.18 | 0.05 | 0.16 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG22 | 4 | 0.18 | 0.05 | 0.16 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG23 | 4 | 0.18 | 0.05 | 0.16 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG21 | 4 | 0.18 | 0.02 | 0.17 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG22 | 4 | 0.18 | 0.02 | 0.17 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG23 | 4 | 0.18 | 0.02 | 0.17 |
| (1,439) | 1:A:111:VAL:HG21 | 1:A:155:SER:HB2 | 4 | 0.17 | 0.01 | 0.17 |
| (1,439) | 1:A:111:VAL:HG22 | 1:A:155:SER:HB2 | 4 | 0.17 | 0.01 | 0.17 |
| (1,439) | 1:A:111:VAL:HG23 | 1:A:155:SER:HB2 | 4 | 0.17 | 0.01 | 0.17 |
| (1,439) | 1:A:111:VAL:HG11 | 1:A:155:SER:HB2 | 4 | 0.17 | 0.01 | 0.17 |
| (1,439) | 1:A:111:VAL:HG12 | 1:A:155:SER:HB2 | 4 | 0.17 | 0.01 | 0.17 |
| (1,439) | 1:A:111:VAL:HG13 | 1:A:155:SER:HB2 | 4 | 0.17 | 0.01 | 0.17 |
| (1,3143) | 1:B:141:LYS:HG3 | 1:B:142:TYR:HB3 | 4 | 0.16 | 0.03 | 0.17 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG2 | 4 | 0.16 | 0.03 | 0.16 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG3 | 4 | 0.16 | 0.03 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG21 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG22 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG23 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG21 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG22 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG23 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG21 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG22 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG23 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG11 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG12 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG13 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG11 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG12 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG13 | 4 | 0.16 | 0.04 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG11 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG12 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG13 | 4 | 0.16 | 0.04 | 0.16 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG21 | 4 | 0.16 | 0.03 | 0.18 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG22 | 4 | 0.16 | 0.03 | 0.18 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG23 | 4 | 0.16 | 0.03 | 0.18 |
| (1,4089) | 1:B:152:GLN:HE22 | 1:B:152:GLN:HB2 | 4 | 0.16 | 0.03 | 0.16 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD11 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD12 | 4 | 0.16 | 0.04 | 0.16 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD13 | 4 | 0.16 | 0.04 | 0.16 |
| (1,419) | 1:A:111:VAL:HA | 1:A:120:ILE:HG13 | 4 | 0.16 | 0.03 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG21 | 4 | 0.16 | 0.01 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG22 | 4 | 0.16 | 0.01 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG23 | 4 | 0.16 | 0.01 | 0.16 |
| (1,857) | 1:A:141:LYS:HG2 | 1:A:143:THR:HA | 4 | 0.15 | 0.03 | 0.14 |
| (1,2892) | 1:B:119:GLU:HA | 1:B:141:LYS:HE2 | 4 | 0.15 | 0.03 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD21 | 4 | 0.15 | 0.01 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD22 | 4 | 0.15 | 0.01 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD23 | 4 | 0.15 | 0.01 | 0.15 |
| (1,2831) | 1:B:117:VAL:HA | 1:B:148:VAL:HB | 4 | 0.15 | 0.02 | 0.16 |
| (1,3015) | 1:B:127:ARG:HA | 1:B:127:ARG:HB3 | 4 | 0.14 | 0.04 | 0.13 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD11 | 4 | 0.14 | 0.03 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD12 | 4 | 0.14 | 0.03 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD13 | 4 | 0.14 | 0.03 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD21 | 4 | 0.14 | 0.03 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD22 | 4 | 0.14 | 0.03 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD23 | 4 | 0.14 | 0.03 | 0.14 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD21 | 4 | 0.14 | 0.03 | 0.14 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD22 | 4 | 0.14 | 0.03 | 0.14 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD23 | 4 | 0.14 | 0.03 | 0.14 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG21 | 4 | 0.14 | 0.02 | 0.15 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG22 | 4 | 0.14 | 0.02 | 0.15 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG23 | 4 | 0.14 | 0.02 | 0.15 |
| (1,2093) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,2093) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,2093) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,2225) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,2225) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,2225) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG3 | 4 | 0.14 | 0.01 | 0.14 |
| (1,3360) | 1:B:153:VAL:HB | 1:B:154:SER:HA | 4 | 0.14 | 0.01 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3292) | 1:B:148:VAL:HG11 | 1:B:169:MET:HA | 4 | 0.14 | 0.02 | 0.14 |
| (1,3292) | 1:B:148:VAL:HG12 | 1:B:169:MET:HA | 4 | 0.14 | 0.02 | 0.14 |
| (1,3292) | 1:B:148:VAL:HG13 | 1:B:169:MET:HA | 4 | 0.14 | 0.02 | 0.14 |
| (1,3438) | 1:B:157:LEU:HB3 | 1:B:157:LEU:HG | 4 | 0.14 | 0.01 | 0.14 |
| (1,1172) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB2 | 4 | 0.13 | 0.02 | 0.12 |
| (1,1172) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB2 | 4 | 0.13 | 0.02 | 0.12 |
| (1,1172) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB2 | 4 | 0.13 | 0.02 | 0.12 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD11 | 4 | 0.13 | 0.02 | 0.13 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD12 | 4 | 0.13 | 0.02 | 0.13 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD13 | 4 | 0.13 | 0.02 | 0.13 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD21 | 4 | 0.13 | 0.01 | 0.12 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD22 | 4 | 0.13 | 0.01 | 0.12 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD23 | 4 | 0.13 | 0.01 | 0.12 |
| (1,1345) | 1:A:97:VAL:H | 1:A:165:VAL:H | 4 | 0.13 | 0.01 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD11 | 4 | 0.13 | 0.01 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD12 | 4 | 0.13 | 0.01 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD13 | 4 | 0.13 | 0.01 | 0.12 |
| (1,3928) | 1:B:132:GLY:H | 1:B:131:HIS:HB3 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1627) | 1:A:129:ASP:H | 1:A:132:GLY:H | 4 | 0.12 | 0.01 | 0.12 |
| (1,2290) | 1:B:90:HIS:HB3 | 1:B:91:THR:HA | 3 | 0.93 | 0.31 | 0.83 |
| (1,841) | 1:A:140:ARG:HG2 | 1:A:142:TYR:HE1 | 3 | 0.82 | 0.51 | 0.58 |
| (1,841) | 1:A:140:ARG:HG2 | 1:A:142:TYR:HE2 | 3 | 0.82 | 0.51 | 0.58 |
| (1,3601) | 1:B:94:ARG:H | 1:B:92:ALA:HA | 3 | 0.81 | 0.55 | 0.45 |
| (1,4285) | 1:B:171:LYS:H | 1:B:169:MET:HA | 3 | 0.79 | 0.38 | 0.65 |
| (1,4293) | 1:B:172:LEU:H | 1:B:171:LYS:HA | 3 | 0.73 | 0.26 | 0.85 |
| (1,4272) | 1:B:169:MET:H | 1:B:95:TRP:HA | 3 | 0.67 | 0.16 | 0.76 |
| (1,4080) | 1:B:152:GLN:HE21 | 1:B:152:GLN:HB3 | 3 | 0.65 | 0.09 | 0.61 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB1 | 3 | 0.6 | 0.31 | 0.4 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB2 | 3 | 0.6 | 0.31 | 0.4 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB3 | 3 | 0.6 | 0.31 | 0.4 |
| (1,3303) | 1:B:148:VAL:HG21 | 1:B:170:PRO:HG2 | 3 | 0.59 | 0.22 | 0.46 |
| (1,3303) | 1:B:148:VAL:HG22 | 1:B:170:PRO:HG2 | 3 | 0.59 | 0.22 | 0.46 |
| (1,3303) | 1:B:148:VAL:HG23 | 1:B:170:PRO:HG2 | 3 | 0.59 | 0.22 | 0.46 |
| (1,2346) | 1:B:95:TRP:HB3 | 1:B:95:TRP:HE3 | 3 | 0.56 | 0.03 | 0.57 |
| (1,65) | 1:A:95:TRP:HB3 | 1:A:95:TRP:HE3 | 3 | 0.56 | 0.01 | 0.56 |
| (1,4048) | 1:B:149:ASP:H | 1:B:170:PRO:HG3 | 3 | 0.53 | 0.2 | 0.62 |
| (1,3603) | 1:B:94:ARG:H | 1:B:93:ASP:HB2 | 3 | 0.53 | 0.09 | 0.54 |
| (1,2513) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HG12 | 3 | 0.49 | 0.09 | 0.43 |
| (1,2513) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HG12 | 3 | 0.49 | 0.09 | 0.43 |
| (1,2513) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HG12 | 3 | 0.49 | 0.09 | 0.43 |
| (1,3557) | 1:B:168:PRO:HA | 1:B:169:MET:HG2 | 3 | 0.47 | 0.4 | 0.23 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG21 | 3 | 0.47 | 0.26 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG22 | 3 | 0.47 | 0.26 | 0.42 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG23 | 3 | 0.47 | 0.26 | 0.42 |
| (1,1331) | 1:A:95:TRP:H | 1:A:95:TRP:HB2 | 3 | 0.46 | 0.04 | 0.47 |
| (1,3613) | 1:B:95:TRP:H | 1:B:95:TRP:HE3 | 3 | 0.43 | 0.08 | 0.45 |
| (1,18) | 1:A:93:ASP:HB2 | 1:A:94:ARG:HA | 3 | 0.42 | 0.12 | 0.5 |
| (1,3096) | 1:B:136:ARG:HG3 | 1:B:138:PHE:HA | 3 | 0.42 | 0.19 | 0.32 |
| (1,1640) | 1:A:132:GLY:H | 1:A:128:GLN:HG2 | 3 | 0.41 | 0.07 | 0.44 |
| (1,1332) | 1:A:95:TRP:H | 1:A:95:TRP:HE3 | 3 | 0.4 | 0.03 | 0.41 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD21 | 3 | 0.38 | 0.09 | 0.38 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD22 | 3 | 0.38 | 0.09 | 0.38 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD23 | 3 | 0.38 | 0.09 | 0.38 |
| (1,704) | 1:A:125:GLU:HA | 1:A:135:SER:HB3 | 3 | 0.37 | 0.35 | 0.13 |
| (1,1974) | 1:A:167:ALA:H | 1:A:95:TRP:HB3 | 3 | 0.37 | 0.04 | 0.36 |
| (1,33) | 1:A:94:ARG:HA | 1:A:169:MET:HB2 | 3 | 0.35 | 0.18 | 0.37 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB1 | 3 | 0.35 | 0.21 | 0.3 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB2 | 3 | 0.35 | 0.21 | 0.3 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB3 | 3 | 0.35 | 0.21 | 0.3 |
| (1,3092) | 1:B:136:ARG:HA | 1:B:136:ARG:HG2 | 3 | 0.35 | 0.06 | 0.38 |
| (1,1924) | 1:A:162:THR:H | 1:A:160:GLU:HB2 | 3 | 0.35 | 0.11 | 0.4 |
| (1,612) | 1:A:119:GLU:HA | 1:A:141:LYS:HE3 | 3 | 0.33 | 0.1 | 0.33 |
| (1,847) | 1:A:141:LYS:HA | 1:A:141:LYS:HE3 | 3 | 0.33 | 0.03 | 0.34 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG21 | 3 | 0.32 | 0.05 | 0.29 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG22 | 3 | 0.32 | 0.05 | 0.29 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG23 | 3 | 0.32 | 0.05 | 0.29 |
| (1,3304) | 1:B:149:ASP:HA | 1:B:149:ASP:HB3 | 3 | 0.32 | 0.1 | 0.35 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD21 | 3 | 0.32 | 0.07 | 0.29 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD22 | 3 | 0.32 | 0.07 | 0.29 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD23 | 3 | 0.32 | 0.07 | 0.29 |
| (1,1321) | 1:A:94:ARG:H | 1:A:93:ASP:HA | 3 | 0.31 | 0.06 | 0.34 |
| (1,1514) | 1:A:118:VAL:H | 1:A:119:GLU:HG3 | 3 | 0.31 | 0.16 | 0.21 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG21 | 3 | 0.3 | 0.11 | 0.23 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG22 | 3 | 0.3 | 0.11 | 0.23 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG23 | 3 | 0.3 | 0.11 | 0.23 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG21 | 3 | 0.29 | 0.12 | 0.36 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG22 | 3 | 0.29 | 0.12 | 0.36 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG23 | 3 | 0.29 | 0.12 | 0.36 |
| (1,336) | 1:A:108:GLU:HA | 1:A:108:GLU:HG2 | 3 | 0.29 | 0.05 | 0.28 |
| (1,3060) | 1:B:131:HIS:HA | 1:B:131:HIS:HE1 | 3 | 0.29 | 0.08 | 0.33 |
| (1,1179) | 1:A:157:LEU:HD21 | 1:A:163:LEU:HB3 | 3 | 0.28 | 0.03 | 0.26 |
| (1,1179) | 1:A:157:LEU:HD22 | 1:A:163:LEU:HB3 | 3 | 0.28 | 0.03 | 0.26 |
| (1,1179) | 1:A:157:LEU:HD23 | 1:A:163:LEU:HB3 | 3 | 0.28 | 0.03 | 0.26 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD21 | 3 | 0.28 | 0.08 | 0.23 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD22 | 3 | 0.28 | 0.08 | 0.23 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD23 | 3 | 0.28 | 0.08 | 0.23 |
| (1,808) | 1:A:135:SER:HA | 1:A:135:SER:HB2 | 3 | 0.27 | 0.01 | 0.27 |
| (1,3607) | 1:B:94:ARG:H | 1:B:168:PRO:HA | 3 | 0.27 | 0.12 | 0.19 |
| (1,917) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA2 | 3 | 0.27 | 0.11 | 0.27 |
| (1,3395) | 1:B:155:SER:HB2 | 1:B:163:LEU:HA | 3 | 0.26 | 0.11 | 0.27 |
| (1,4281) | 1:B:169:MET:H | 1:B:169:MET:HG3 | 3 | 0.25 | 0.05 | 0.25 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD21 | 3 | 0.24 | 0.0 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD22 | 3 | 0.24 | 0.0 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD23 | 3 | 0.24 | 0.0 | 0.24 |
| (1,3366) | 1:B:153:VAL:HG11 | 1:B:155:SER:HB3 | 3 | 0.24 | 0.06 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG12 | 1:B:155:SER:HB3 | 3 | 0.24 | 0.06 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG13 | 1:B:155:SER:HB3 | 3 | 0.24 | 0.06 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG21 | 1:B:155:SER:HB3 | 3 | 0.24 | 0.06 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG22 | 1:B:155:SER:HB3 | 3 | 0.24 | 0.06 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG23 | 1:B:155:SER:HB3 | 3 | 0.24 | 0.06 | 0.28 |
| (1,434) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG12 | 3 | 0.24 | 0.02 | 0.24 |
| (1,434) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG12 | 3 | 0.24 | 0.02 | 0.24 |
| (1,434) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG12 | 3 | 0.24 | 0.02 | 0.24 |
| (1,434) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG12 | 3 | 0.24 | 0.02 | 0.24 |
| (1,434) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG12 | 3 | 0.24 | 0.02 | 0.24 |
| (1,434) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG12 | 3 | 0.24 | 0.02 | 0.24 |
| (1,746) | 1:A:128:GLN:HA | 1:A:128:GLN:HG3 | 3 | 0.24 | 0.05 | 0.2 |
| (1,93) | 1:A:96:ARG:HB2 | 1:A:96:ARG:HD3 | 3 | 0.23 | 0.02 | 0.21 |
| (1,93) | 1:A:96:ARG:HB2 | 1:A:96:ARG:HD2 | 3 | 0.23 | 0.02 | 0.21 |
| (1,2715) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG12 | 3 | 0.23 | 0.07 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG12 | 3 | 0.23 | 0.07 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG12 | 3 | 0.23 | 0.07 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG12 | 3 | 0.23 | 0.07 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG12 | 3 | 0.23 | 0.07 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG12 | 3 | 0.23 | 0.07 | 0.2 |
| (1,2891) | 1:B:119:GLU:HA | 1:B:141:LYS:HD3 | 3 | 0.23 | 0.05 | 0.2 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD21 | 3 | 0.22 | 0.01 | 0.23 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD22 | 3 | 0.22 | 0.01 | 0.23 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD23 | 3 | 0.22 | 0.01 | 0.23 |
| (1,862) | 1:A:141:LYS:HG3 | 1:A:142:TYR:HB3 | 3 | 0.21 | 0.04 | 0.24 |
| (1,749) | 1:A:128:GLN:HA | 1:A:133:TYR:HE1 | 3 | 0.21 | 0.03 | 0.2 |
| (1,749) | 1:A:128:GLN:HA | 1:A:133:TYR:HE2 | 3 | 0.21 | 0.03 | 0.2 |
| (1,2329) | 1:B:94:ARG:HD2 | 1:B:168:PRO:HA | 3 | 0.21 | 0.07 | 0.19 |
| (1,3539) | 1:B:166:GLU:HG2 | 1:B:167:ALA:HA | 3 | 0.21 | 0.05 | 0.22 |
| (1,3539) | 1:B:166:GLU:HG3 | 1:B:167:ALA:HA | 3 | 0.21 | 0.05 | 0.22 |
| (1,3654) | 1:B:102:ASN:HD21 | 1:B:161:GLY:HA2 | 3 | 0.21 | 0.06 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3795) | 1:B:118:VAL:H | 1:B:119:GLU:HG3 | 3 | 0.21 | 0.01 | 0.21 |
| (1,1014) | 1:A:148:VAL:HG11 | 1:A:170:PRO:HG3 | 3 | 0.2 | 0.02 | 0.2 |
| (1,1014) | 1:A:148:VAL:HG12 | 1:A:170:PRO:HG3 | 3 | 0.2 | 0.02 | 0.2 |
| (1,1014) | 1:A:148:VAL:HG13 | 1:A:170:PRO:HG3 | 3 | 0.2 | 0.02 | 0.2 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD11 | 3 | 0.2 | 0.05 | 0.2 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD12 | 3 | 0.2 | 0.05 | 0.2 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD13 | 3 | 0.2 | 0.05 | 0.2 |
| (1,773) | 1:A:130:GLU:HA | 1:A:130:GLU:HG3 | 3 | 0.2 | 0.03 | 0.2 |
| (1,1327) | 1:A:94:ARG:H | 1:A:169:MET:HG2 | 3 | 0.2 | 0.06 | 0.22 |
| (1,3664) | 1:B:102:ASN:HD22 | 1:B:161:GLY:HA3 | 3 | 0.2 | 0.03 | 0.21 |
| (1,3918) | 1:B:131:HIS:H | 1:B:130:GLU:HG2 | 3 | 0.19 | 0.06 | 0.19 |
| (1,3918) | 1:B:131:HIS:H | 1:B:130:GLU:HG3 | 3 | 0.19 | 0.06 | 0.19 |
| (1,1276) | 1:A:168:PRO:HA | 1:A:169:MET:HG2 | 3 | 0.19 | 0.07 | 0.18 |
| (1,1637) | 1:A:131:HIS:H | 1:A:130:GLU:HG2 | 3 | 0.19 | 0.06 | 0.23 |
| (1,1637) | 1:A:131:HIS:H | 1:A:130:GLU:HG3 | 3 | 0.19 | 0.06 | 0.23 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD11 | 3 | 0.19 | 0.05 | 0.18 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD12 | 3 | 0.19 | 0.05 | 0.18 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD13 | 3 | 0.19 | 0.05 | 0.18 |
| (1,700) | 1:A:125:GLU:HA | 1:A:125:GLU:HG3 | 3 | 0.19 | 0.03 | 0.2 |
| (1,1383) | 1:A:102:ASN:HD22 | 1:A:161:GLY:HA3 | 3 | 0.19 | 0.04 | 0.19 |
| (1,3663) | 1:B:102:ASN:HD22 | 1:B:161:GLY:HA2 | 3 | 0.19 | 0.02 | 0.18 |
| (1,737) | 1:A:127:ARG:HA | 1:A:127:ARG:HD3 | 3 | 0.18 | 0.05 | 0.21 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD11 | 3 | 0.18 | 0.03 | 0.19 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD12 | 3 | 0.18 | 0.03 | 0.19 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD13 | 3 | 0.18 | 0.03 | 0.19 |
| (1,2310) | 1:B:94:ARG:HA | 1:B:168:PRO:HA | 3 | 0.18 | 0.04 | 0.18 |
| (1,2791) | 1:B:114:LYS:HB2 | 1:B:118:VAL:HA | 3 | 0.18 | 0.03 | 0.2 |
| (1,2791) | 1:B:114:LYS:HB3 | 1:B:118:VAL:HA | 3 | 0.18 | 0.03 | 0.2 |
| (1,1591) | 1:A:126:GLU:H | 1:A:135:SER:HB2 | 3 | 0.18 | 0.06 | 0.18 |
| (1,1591) | 1:A:126:GLU:H | 1:A:135:SER:HB3 | 3 | 0.18 | 0.06 | 0.18 |
| (1,3614) | 1:B:95:TRP:H | 1:B:166:GLU:HG2 | 3 | 0.18 | 0.06 | 0.14 |
| (1,3614) | 1:B:95:TRP:H | 1:B:166:GLU:HG3 | 3 | 0.18 | 0.06 | 0.14 |
| (1,3699) | 1:B:108:GLU:H | 1:B:108:GLU:HG2 | 3 | 0.18 | 0.03 | 0.16 |
| (1,3699) | 1:B:108:GLU:H | 1:B:108:GLU:HG3 | 3 | 0.18 | 0.03 | 0.16 |
| (1,4196) | 1:B:162:THR:H | 1:B:102:ASN:HB2 | 3 | 0.18 | 0.04 | 0.18 |
| (1,1545) | 1:A:120:ILE:H | 1:A:140:ARG:HG3 | 3 | 0.18 | 0.04 | 0.2 |
| (1,2518) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HB | 3 | 0.18 | 0.01 | 0.17 |
| (1,2518) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HB | 3 | 0.18 | 0.01 | 0.17 |
| (1,2518) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HB | 3 | 0.18 | 0.01 | 0.17 |
| (1,2918) | 1:B:120:ILE:HB | 1:B:142:TYR:HE1 | 3 | 0.18 | 0.04 | 0.15 |
| (1,2918) | 1:B:120:ILE:HB | 1:B:142:TYR:HE2 | 3 | 0.18 | 0.04 | 0.15 |
| (1,1489) | 1:A:114:LYS:H | 1:A:119:GLU:H | 3 | 0.17 | 0.02 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB1 | 3 | 0.17 | 0.06 | 0.15 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB2 | 3 | 0.17 | 0.06 | 0.15 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB3 | 3 | 0.17 | 0.06 | 0.15 |
| (1,2578) | 1:B:105:ALA:HB1 | 1:B:107:ASP:HB3 | 3 | 0.17 | 0.05 | 0.18 |
| (1,2578) | 1:B:105:ALA:HB2 | 1:B:107:ASP:HB3 | 3 | 0.17 | 0.05 | 0.18 |
| (1,2578) | 1:B:105:ALA:HB3 | 1:B:107:ASP:HB3 | 3 | 0.17 | 0.05 | 0.18 |
| (1,849) | 1:A:141:LYS:HB2 | 1:A:141:LYS:HE2 | 3 | 0.17 | 0.03 | 0.18 |
| (1,3133) | 1:B:141:LYS:HG2 | 1:B:141:LYS:HE2 | 3 | 0.17 | 0.03 | 0.17 |
| (1,1517) | 1:A:118:VAL:H | 1:A:142:TYR:HB2 | 3 | 0.16 | 0.04 | 0.15 |
| (1,3872) | 1:B:126:GLU:H | 1:B:135:SER:HB2 | 3 | 0.16 | 0.05 | 0.15 |
| (1,3872) | 1:B:126:GLU:H | 1:B:135:SER:HB3 | 3 | 0.16 | 0.05 | 0.15 |
| (1,1373) | 1:A:102:ASN:HD21 | 1:A:161:GLY:HA2 | 3 | 0.16 | 0.02 | 0.15 |
| (1,1581) | 1:A:125:GLU:H | 1:A:108:GLU:HG3 | 3 | 0.16 | 0.05 | 0.14 |
| (1,1611) | 1:A:128:GLN:HE22 | 1:A:128:GLN:H | 3 | 0.16 | 0.04 | 0.15 |
| (1,2028) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB3 | 3 | 0.16 | 0.0 | 0.16 |
| (1,2160) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB3 | 3 | 0.16 | 0.0 | 0.16 |
| (1,331) | 1:A:107:ASP:HA | 1:A:108:GLU:HG2 | 3 | 0.15 | 0.02 | 0.16 |
| (1,4183) | 1:B:161:GLY:H | 1:B:102:ASN:HB3 | 3 | 0.15 | 0.03 | 0.14 |
| (1,3770) | 1:B:114:LYS:H | 1:B:119:GLU:H | 3 | 0.15 | 0.01 | 0.16 |
| (1,395) | 1:A:110:THR:HB | 1:A:112:LYS:HG2 | 3 | 0.15 | 0.03 | 0.15 |
| (1,395) | 1:A:110:THR:HB | 1:A:112:LYS:HG3 | 3 | 0.15 | 0.03 | 0.15 |
| (1,101) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HA | 3 | 0.15 | 0.03 | 0.16 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB1 | 3 | 0.15 | 0.03 | 0.16 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB2 | 3 | 0.15 | 0.03 | 0.16 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB3 | 3 | 0.15 | 0.03 | 0.16 |
| (1,1389) | 1:A:105:ALA:H | 1:A:106:PRO:HD3 | 3 | 0.14 | 0.02 | 0.15 |
| (1,1964) | 1:A:166:GLU:H | 1:A:155:SER:HB2 | 3 | 0.14 | 0.02 | 0.15 |
| (1,1964) | 1:A:166:GLU:H | 1:A:155:SER:HB3 | 3 | 0.14 | 0.02 | 0.15 |
| (1,3037) | 1:B:128:GLN:HB3 | 1:B:133:TYR:HD1 | 3 | 0.14 | 0.03 | 0.13 |
| (1,3037) | 1:B:128:GLN:HB3 | 1:B:133:TYR:HD2 | 3 | 0.14 | 0.03 | 0.13 |
| (1,1096) | 1:A:154:SER:HB2 | 1:A:166:GLU:HG3 | 3 | 0.14 | 0.0 | 0.14 |
| (1,1096) | 1:A:154:SER:HB2 | 1:A:166:GLU:HG2 | 3 | 0.14 | 0.0 | 0.14 |
| (1,3869) | 1:B:126:GLU:H | 1:B:125:GLU:HG3 | 3 | 0.14 | 0.02 | 0.14 |
| (1,413) | 1:A:111:VAL:HA | 1:A:112:LYS:HG2 | 3 | 0.14 | 0.03 | 0.13 |
| (1,413) | 1:A:111:VAL:HA | 1:A:112:LYS:HG3 | 3 | 0.14 | 0.03 | 0.13 |
| (1,779) | 1:A:131:HIS:HA | 1:A:131:HIS:HE1 | 3 | 0.14 | 0.02 | 0.15 |
| (1,1576) | 1:A:124:HIS:H | 1:A:136:ARG:HA | 3 | 0.14 | 0.04 | 0.11 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG21 | 3 | 0.14 | 0.03 | 0.12 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG22 | 3 | 0.14 | 0.03 | 0.12 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG23 | 3 | 0.14 | 0.03 | 0.12 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG21 | 3 | 0.14 | 0.03 | 0.12 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG22 | 3 | 0.14 | 0.03 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG23 | 3 | 0.14 | 0.03 | 0.12 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG21 | 3 | 0.14 | 0.02 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG22 | 3 | 0.14 | 0.02 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG23 | 3 | 0.14 | 0.02 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG11 | 3 | 0.14 | 0.02 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG12 | 3 | 0.14 | 0.02 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG13 | 3 | 0.14 | 0.02 | 0.14 |
| (1,3455) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HG | 3 | 0.13 | 0.03 | 0.12 |
| (1,3455) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HG | 3 | 0.13 | 0.03 | 0.12 |
| (1,3455) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HG | 3 | 0.13 | 0.03 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG21 | 3 | 0.13 | 0.03 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG22 | 3 | 0.13 | 0.03 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG23 | 3 | 0.13 | 0.03 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG11 | 3 | 0.13 | 0.03 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG12 | 3 | 0.13 | 0.03 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG13 | 3 | 0.13 | 0.03 | 0.12 |
| (1,2352) | 1:B:95:TRP:HB2 | 1:B:168:PRO:HB2 | 3 | 0.13 | 0.0 | 0.13 |
| (1,2352) | 1:B:95:TRP:HB3 | 1:B:168:PRO:HB2 | 3 | 0.13 | 0.0 | 0.13 |
| (1,2886) | 1:B:119:GLU:HA | 1:B:120:ILE:HG13 | 3 | 0.13 | 0.02 | 0.12 |
| (1,236) | 1:A:99:LEU:HD11 | 1:A:164:THR:HA | 3 | 0.13 | 0.01 | 0.13 |
| (1,236) | 1:A:99:LEU:HD12 | 1:A:164:THR:HA | 3 | 0.13 | 0.01 | 0.13 |
| (1,236) | 1:A:99:LEU:HD13 | 1:A:164:THR:HA | 3 | 0.13 | 0.01 | 0.13 |
| (1,571) | 1:A:118:VAL:HB | 1:A:142:TYR:HD1 | 3 | 0.13 | 0.01 | 0.13 |
| (1,571) | 1:A:118:VAL:HB | 1:A:142:TYR:HD2 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD11 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD12 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD13 | 3 | 0.13 | 0.01 | 0.13 |
| (1,161) | 1:A:97:VAL:HG21 | 1:A:166:GLU:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,161) | 1:A:97:VAL:HG22 | 1:A:166:GLU:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,161) | 1:A:97:VAL:HG23 | 1:A:166:GLU:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,1870) | 1:A:157:LEU:H | 1:A:157:LEU:HB3 | 3 | 0.12 | 0.01 | 0.12 |
| (1,2798) | 1:B:115:ASP:HB3 | 1:B:150:PRO:HG2 | 3 | 0.12 | 0.0 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG21 | 3 | 0.12 | 0.0 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG22 | 3 | 0.12 | 0.0 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG23 | 3 | 0.12 | 0.0 | 0.12 |
| (1,4043) | 1:B:149:ASP:H | 1:B:152:GLN:HB2 | 3 | 0.12 | 0.01 | 0.13 |
| (1,759) | 1:A:128:GLN:HG2 | 1:A:133:TYR:HA | 3 | 0.12 | 0.01 | 0.11 |
| (1,1849) | 1:A:155:SER:H | 1:A:156:SER:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG11 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG12 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG13 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG21 | 3 | 0.12 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG22 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG23 | 3 | 0.12 | 0.01 | 0.12 |
| (1,3670) | 1:B:105:ALA:H | 1:B:106:PRO:HD3 | 3 | 0.12 | 0.0 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG21 | 3 | 0.12 | 0.0 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG22 | 3 | 0.12 | 0.0 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG23 | 3 | 0.12 | 0.0 | 0.12 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG11 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG12 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG13 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG21 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG22 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG23 | 3 | 0.11 | 0.0 | 0.11 |
| (1,2302) | 1:B:93:ASP:HB3 | 1:B:94:ARG:HG2 | 2 | 1.48 | 0.17 | 1.48 |
| (1,1614) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB2 | 2 | 0.9 | 0.23 | 0.9 |
| (1,2012) | 1:A:172:LEU:H | 1:A:171:LYS:HA | 2 | 0.9 | 0.07 | 0.9 |
| (1,3271) | 1:B:148:VAL:HA | 1:B:169:MET:HB2 | 2 | 0.87 | 0.11 | 0.87 |
| (1,3293) | 1:B:148:VAL:HG11 | 1:B:169:MET:HB2 | 2 | 0.7 | 0.14 | 0.7 |
| (1,3293) | 1:B:148:VAL:HG12 | 1:B:169:MET:HB2 | 2 | 0.7 | 0.14 | 0.7 |
| (1,3293) | 1:B:148:VAL:HG13 | 1:B:169:MET:HB2 | 2 | 0.7 | 0.14 | 0.7 |
| (1,1318) | 1:A:171:LYS:HA | 1:A:171:LYS:HD2 | 2 | 0.67 | 0.04 | 0.67 |
| (1,1318) | 1:A:171:LYS:HA | 1:A:171:LYS:HD3 | 2 | 0.67 | 0.04 | 0.67 |
| (1,1482) | 1:A:114:LYS:H | 1:A:115:ASP:HB2 | 2 | 0.62 | 0.19 | 0.62 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG21 | 2 | 0.58 | 0.41 | 0.58 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG22 | 2 | 0.58 | 0.41 | 0.58 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG23 | 2 | 0.58 | 0.41 | 0.58 |
| (1,2545) | 1:B:100:ASP:HB2 | 1:B:162:THR:HB | 2 | 0.56 | 0.13 | 0.56 |
| (1,4065) | 1:B:152:GLN:H | 1:B:149:ASP:HB3 | 2 | 0.55 | 0.24 | 0.55 |
| (1,2991) | 1:B:126:GLU:HA | 1:B:135:SER:HB2 | 2 | 0.52 | 0.29 | 0.52 |
| (1,770) | 1:A:129:ASP:HB3 | 1:A:130:GLU:HA | 2 | 0.52 | 0.04 | 0.52 |
| (1,1608) | 1:A:128:GLN:HE22 | 1:A:128:GLN:HB2 | 2 | 0.46 | 0.27 | 0.46 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG21 | 2 | 0.46 | 0.18 | 0.46 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG22 | 2 | 0.46 | 0.18 | 0.46 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG23 | 2 | 0.46 | 0.18 | 0.46 |
| (1,2068) | 1:B:134:ILE:HG21 | 1:A:140:ARG:HD3 | 2 | 0.43 | 0.09 | 0.43 |
| (1,2068) | 1:B:134:ILE:HG22 | 1:A:140:ARG:HD3 | 2 | 0.43 | 0.09 | 0.43 |
| (1,2068) | 1:B:134:ILE:HG23 | 1:A:140:ARG:HD3 | 2 | 0.43 | 0.09 | 0.43 |
| (1,2200) | 1:B:134:ILE:HG21 | 1:A:140:ARG:HD3 | 2 | 0.43 | 0.09 | 0.43 |
| (1,2200) | 1:B:134:ILE:HG22 | 1:A:140:ARG:HD3 | 2 | 0.43 | 0.09 | 0.43 |
| (1,2200) | 1:B:134:ILE:HG23 | 1:A:140:ARG:HD3 | 2 | 0.43 | 0.09 | 0.43 |
| (1,1920) | 1:A:162:THR:H | 1:A:158:SER:HB2 | 2 | 0.42 | 0.24 | 0.42 |
| (1,4286) | 1:B:171:LYS:H | 1:B:170:PRO:HB2 | 2 | 0.42 | 0.22 | 0.42 |
| (1,4286) | 1:B:171:LYS:H | 1:B:170:PRO:HB3 | 2 | 0.42 | 0.22 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2008) | 1:A:171:LYS:H | 1:A:171:LYS:HA | 2 | 0.42 | 0.01 | 0.42 |
| (1,2313) | 1:B:94:ARG:HA | 1:B:168:PRO:HD3 | 2 | 0.41 | 0.14 | 0.41 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD21 | 2 | 0.4 | 0.02 | 0.4 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD22 | 2 | 0.4 | 0.02 | 0.4 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD23 | 2 | 0.4 | 0.02 | 0.4 |
| (1,4037) | 1:B:148:VAL:H | 1:B:170:PRO:HG3 | 2 | 0.4 | 0.01 | 0.4 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG21 | 2 | 0.38 | 0.05 | 0.38 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG22 | 2 | 0.38 | 0.05 | 0.38 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG23 | 2 | 0.38 | 0.05 | 0.38 |
| (1,1656) | 1:A:134:ILE:H | 1:A:127:ARG:HG3 | 2 | 0.36 | 0.24 | 0.36 |
| (1,4036) | 1:B:148:VAL:H | 1:B:170:PRO:HB2 | 2 | 0.35 | 0.19 | 0.35 |
| (1,247) | 1:A:99:LEU:HD21 | 1:A:140:ARG:HG3 | 2 | 0.34 | 0.1 | 0.34 |
| (1,247) | 1:A:99:LEU:HD22 | 1:A:140:ARG:HG3 | 2 | 0.34 | 0.1 | 0.34 |
| (1,247) | 1:A:99:LEU:HD23 | 1:A:140:ARG:HG3 | 2 | 0.34 | 0.1 | 0.34 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD21 | 2 | 0.33 | 0.01 | 0.33 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD22 | 2 | 0.33 | 0.01 | 0.33 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD23 | 2 | 0.33 | 0.01 | 0.33 |
| (1,3889) | 1:B:128:GLN:HE22 | 1:B:128:GLN:HB2 | 2 | 0.33 | 0.18 | 0.33 |
| (1,1767) | 1:A:149:ASP:H | 1:A:170:PRO:HG3 | 2 | 0.32 | 0.13 | 0.32 |
| (1,2529) | 1:B:99:LEU:HD21 | 1:B:140:ARG:HD2 | 2 | 0.32 | 0.06 | 0.32 |
| (1,2529) | 1:B:99:LEU:HD22 | 1:B:140:ARG:HD2 | 2 | 0.32 | 0.06 | 0.32 |
| (1,2529) | 1:B:99:LEU:HD23 | 1:B:140:ARG:HD2 | 2 | 0.32 | 0.06 | 0.32 |
| (1,3027) | 1:B:128:GLN:HA | 1:B:128:GLN:HG3 | 2 | 0.32 | 0.15 | 0.32 |
| (1,1323) | 1:A:94:ARG:H | 1:A:93:ASP:HB3 | 2 | 0.3 | 0.01 | 0.3 |
| (1,1326) | 1:A:94:ARG:H | 1:A:168:PRO:HA | 2 | 0.3 | 0.08 | 0.3 |
| (1,3602) | 1:B:94:ARG:H | 1:B:93:ASP:HA | 2 | 0.29 | 0.03 | 0.29 |
| (1,3862) | 1:B:125:GLU:H | 1:B:108:GLU:HG3 | 2 | 0.29 | 0.02 | 0.29 |
| (1,1915) | 1:A:162:THR:H | 1:A:102:ASN:HB2 | 2 | 0.28 | 0.02 | 0.28 |
| (1,19) | 1:A:93:ASP:HB2 | 1:A:94:ARG:HG2 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3014) | 1:B:126:GLU:HG3 | 1:B:135:SER:HB3 | 2 | 0.28 | 0.1 | 0.28 |
| (1,264) | 1:A:100:ASP:HB2 | 1:A:162:THR:HB | 2 | 0.26 | 0.12 | 0.26 |
| (1,635) | 1:A:120:ILE:HB | 1:A:140:ARG:HD2 | 2 | 0.26 | 0.06 | 0.26 |
| (1,1650) | 1:A:132:GLY:H | 1:A:133:TYR:HD1 | 2 | 0.26 | 0.03 | 0.26 |
| (1,1650) | 1:A:132:GLY:H | 1:A:133:TYR:HD2 | 2 | 0.26 | 0.03 | 0.26 |
| (1,2060) | 1:B:134:ILE:HA | 1:A:140:ARG:HG3 | 2 | 0.26 | 0.02 | 0.26 |
| (1,2192) | 1:B:134:ILE:HA | 1:A:140:ARG:HG3 | 2 | 0.26 | 0.02 | 0.26 |
| (1,703) | 1:A:125:GLU:HA | 1:A:135:SER:HB2 | 2 | 0.24 | 0.08 | 0.24 |
| (1,2626) | 1:B:108:GLU:HG2 | 1:B:123:LYS:HE3 | 2 | 0.24 | 0.13 | 0.24 |
| (1,2626) | 1:B:108:GLU:HG2 | 1:B:123:LYS:HE2 | 2 | 0.24 | 0.13 | 0.24 |
| (1,3865) | 1:B:125:GLU:H | 1:B:126:GLU:H | 2 | 0.24 | 0.0 | 0.24 |
| (1,2965) | 1:B:123:LYS:HA | 1:B:135:SER:HB3 | 2 | 0.24 | 0.02 | 0.24 |
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG21 | 2 | 0.24 | 0.0 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG22 | 2 | 0.24 | 0.0 | 0.24 |
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG23 | 2 | 0.24 | 0.0 | 0.24 |
| (1,3908) | 1:B:129:ASP:H | 1:B:132:GLY:H | 2 | 0.24 | 0.02 | 0.24 |
| (1,346) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HG3 | 2 | 0.23 | 0.05 | 0.23 |
| (1,346) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HG2 | 2 | 0.23 | 0.05 | 0.23 |
| (1,1584) | 1:A:125:GLU:H | 1:A:126:GLU:H | 2 | 0.23 | 0.04 | 0.23 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG11 | 2 | 0.22 | 0.04 | 0.22 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG12 | 2 | 0.22 | 0.04 | 0.22 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG13 | 2 | 0.22 | 0.04 | 0.22 |
| (1,4052) | 1:B:151:THR:H | 1:B:149:ASP:HB3 | 2 | 0.22 | 0.01 | 0.22 |
| (1,234) | 1:A:99:LEU:HD11 | 1:A:140:ARG:HD3 | 2 | 0.22 | 0.02 | 0.22 |
| (1,234) | 1:A:99:LEU:HD12 | 1:A:140:ARG:HD3 | 2 | 0.22 | 0.02 | 0.22 |
| (1,234) | 1:A:99:LEU:HD13 | 1:A:140:ARG:HD3 | 2 | 0.22 | 0.02 | 0.22 |
| (1,234) | 1:A:99:LEU:HD11 | 1:A:140:ARG:HD2 | 2 | 0.22 | 0.02 | 0.22 |
| (1,234) | 1:A:99:LEU:HD12 | 1:A:140:ARG:HD2 | 2 | 0.22 | 0.02 | 0.22 |
| (1,234) | 1:A:99:LEU:HD13 | 1:A:140:ARG:HD2 | 2 | 0.22 | 0.02 | 0.22 |
| (1,2330) | 1:B:94:ARG:HD3 | 1:B:168:PRO:HA | 2 | 0.22 | 0.1 | 0.22 |
| (1,3861) | 1:B:125:GLU:H | 1:B:108:GLU:HG2 | 2 | 0.22 | 0.01 | 0.22 |
| (1,3605) | 1:B:94:ARG:H | 1:B:94:ARG:HG2 | 2 | 0.21 | 0.04 | 0.21 |
| (1,3605) | 1:B:94:ARG:H | 1:B:94:ARG:HG3 | 2 | 0.21 | 0.04 | 0.21 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD21 | 2 | 0.21 | 0.05 | 0.21 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD22 | 2 | 0.21 | 0.05 | 0.21 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD23 | 2 | 0.21 | 0.05 | 0.21 |
| (1,2996) | 1:B:126:GLU:HB2 | 1:B:135:SER:HB3 | 2 | 0.21 | 0.03 | 0.21 |
| (1,2996) | 1:B:126:GLU:HB3 | 1:B:135:SER:HB3 | 2 | 0.21 | 0.03 | 0.21 |
| (1,2592) | 1:B:106:PRO:HA | 1:B:109:LEU:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,2981) | 1:B:125:GLU:HA | 1:B:125:GLU:HG3 | 2 | 0.2 | 0.0 | 0.2 |
| (1,3672) | 1:B:105:ALA:H | 1:B:108:GLU:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,2613) | 1:B:107:ASP:HA | 1:B:108:GLU:HG3 | 2 | 0.2 | 0.07 | 0.2 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD11 | 2 | 0.2 | 0.02 | 0.2 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD12 | 2 | 0.2 | 0.02 | 0.2 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD13 | 2 | 0.2 | 0.02 | 0.2 |
| (1,756) | 1:A:128:GLN:HB3 | 1:A:133:TYR:HD1 | 2 | 0.2 | 0.04 | 0.2 |
| (1,756) | 1:A:128:GLN:HB3 | 1:A:133:TYR:HD2 | 2 | 0.2 | 0.04 | 0.2 |
| (1,1128) | 1:A:155:SER:HB3 | 1:A:157:LEU:HB3 | 2 | 0.19 | 0.01 | 0.19 |
| (1,1128) | 1:A:155:SER:HB2 | 1:A:157:LEU:HB3 | 2 | 0.19 | 0.01 | 0.19 |
| (1,3868) | 1:B:126:GLU:H | 1:B:125:GLU:HG2 | 2 | 0.19 | 0.01 | 0.19 |
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD21 | 2 | 0.18 | 0.04 | 0.18 |
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD22 | 2 | 0.18 | 0.04 | 0.18 |
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD23 | 2 | 0.18 | 0.04 | 0.18 |
| (1,717) | 1:A:126:GLU:HG2 | 1:A:127:ARG:HG3 | 2 | 0.18 | 0.04 | 0.18 |
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG21 | 2 | 0.18 | 0.04 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG22 | 2 | 0.18 | 0.04 | 0.18 |
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG23 | 2 | 0.18 | 0.04 | 0.18 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG21 | 2 | 0.18 | 0.04 | 0.18 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG22 | 2 | 0.18 | 0.04 | 0.18 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG23 | 2 | 0.18 | 0.04 | 0.18 |
| (1,296) | 1:A:105:ALA:HB1 | 1:A:107:ASP:HB2 | 2 | 0.18 | 0.0 | 0.18 |
| (1,296) | 1:A:105:ALA:HB2 | 1:A:107:ASP:HB2 | 2 | 0.18 | 0.0 | 0.18 |
| (1,296) | 1:A:105:ALA:HB3 | 1:A:107:ASP:HB2 | 2 | 0.18 | 0.0 | 0.18 |
| (1,649) | 1:A:120:ILE:HG21 | 1:A:140:ARG:HA | 2 | 0.18 | 0.07 | 0.18 |
| (1,649) | 1:A:120:ILE:HG22 | 1:A:140:ARG:HA | 2 | 0.18 | 0.07 | 0.18 |
| (1,649) | 1:A:120:ILE:HG23 | 1:A:140:ARG:HA | 2 | 0.18 | 0.07 | 0.18 |
| (1,1104) | 1:A:155:SER:HA | 1:A:156:SER:HB3 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2756) | 1:B:112:LYS:HE2 | 1:B:119:GLU:HG2 | 2 | 0.18 | 0.03 | 0.18 |
| (1,2756) | 1:B:112:LYS:HE3 | 1:B:119:GLU:HG2 | 2 | 0.18 | 0.03 | 0.18 |
| (1,3641) | 1:B:101:VAL:H | 1:B:100:ASP:HB2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3641) | 1:B:101:VAL:H | 1:B:100:ASP:HB3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,2540) | 1:B:100:ASP:HA | 1:B:100:ASP:HB3 | 2 | 0.18 | 0.03 | 0.18 |
| (1,3000) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HD1 | 2 | 0.18 | 0.0 | 0.18 |
| (1,3000) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HD2 | 2 | 0.18 | 0.0 | 0.18 |
| (1,3521) | 1:B:164:THR:HB | 1:B:166:GLU:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3521) | 1:B:164:THR:HB | 1:B:166:GLU:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,4115) | 1:B:154:SER:H | 1:B:155:SER:HB2 | 2 | 0.18 | 0.03 | 0.18 |
| (1,4194) | 1:B:161:GLY:H | 1:B:162:THR:HB | 2 | 0.18 | 0.0 | 0.18 |
| (1,4290) | 1:B:171:LYS:H | 1:B:171:LYS:HB2 | 2 | 0.18 | 0.04 | 0.18 |
| (1,4290) | 1:B:171:LYS:H | 1:B:171:LYS:HB3 | 2 | 0.18 | 0.04 | 0.18 |
| (1,602) | 1:A:119:GLU:HA | 1:A:119:GLU:HG3 | 2 | 0.17 | 0.0 | 0.17 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD11 | 2 | 0.17 | 0.03 | 0.17 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD12 | 2 | 0.17 | 0.03 | 0.17 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD13 | 2 | 0.17 | 0.03 | 0.17 |
| (1,345) | 1:A:108:GLU:HG2 | 1:A:123:LYS:HE3 | 2 | 0.17 | 0.04 | 0.17 |
| (1,345) | 1:A:108:GLU:HG2 | 1:A:123:LYS:HE2 | 2 | 0.17 | 0.04 | 0.17 |
| (1,610) | 1:A:119:GLU:HA | 1:A:141:LYS:HD3 | 2 | 0.17 | 0.02 | 0.17 |
| (1,1844) | 1:A:154:SER:H | 1:A:168:PRO:HD2 | 2 | 0.17 | 0.05 | 0.17 |
| (1,2559) | 1:B:102:ASN:HB2 | 1:B:161:GLY:HA3 | 2 | 0.17 | 0.04 | 0.17 |
| (1,4076) | 1:B:152:GLN:H | 1:B:170:PRO:HD2 | 2 | 0.17 | 0.02 | 0.17 |
| (1,4076) | 1:B:152:GLN:H | 1:B:170:PRO:HD3 | 2 | 0.17 | 0.02 | 0.17 |
| (1,4125) | 1:B:154:SER:H | 1:B:168:PRO:HD2 | 2 | 0.17 | 0.01 | 0.17 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3093) | 1:B:136:ARG:HA | 1:B:136:ARG:HD2 | 2 | 0.16 | 0.04 | 0.16 |
| (1,4038) | 1:B:148:VAL:H | 1:B:170:PRO:HD2 | 2 | 0.16 | 0.02 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,4038) | 1:B:148:VAL:H | 1:B:170:PRO:HD3 | 2 | 0.16 | 0.02 | 0.16 |
| (1,475) | 1:A:112:LYS:HE2 | 1:A:119:GLU:HG2 | 2 | 0.16 | 0.05 | 0.16 |
| (1,475) | 1:A:112:LYS:HE3 | 1:A:119:GLU:HG2 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD11 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD12 | 2 | 0.16 | 0.05 | 0.16 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD13 | 2 | 0.16 | 0.05 | 0.16 |
| (1,3087) | 1:B:134:ILE:HG21 | 1:B:135:SER:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3087) | 1:B:134:ILE:HG22 | 1:B:135:SER:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3087) | 1:B:134:ILE:HG23 | 1:B:135:SER:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3087) | 1:B:134:ILE:HD11 | 1:B:135:SER:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3087) | 1:B:134:ILE:HD12 | 1:B:135:SER:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3087) | 1:B:134:ILE:HD13 | 1:B:135:SER:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (1,3481) | 1:B:159:PRO:HA | 1:B:159:PRO:HG3 | 2 | 0.16 | 0.05 | 0.16 |
| (1,992) | 1:A:148:VAL:HA | 1:A:170:PRO:HB3 | 2 | 0.16 | 0.02 | 0.16 |
| (1,298) | 1:A:105:ALA:HB1 | 1:A:108:GLU:HB2 | 2 | 0.16 | 0.01 | 0.16 |
| (1,298) | 1:A:105:ALA:HB2 | 1:A:108:GLU:HB2 | 2 | 0.16 | 0.01 | 0.16 |
| (1,298) | 1:A:105:ALA:HB3 | 1:A:108:GLU:HB2 | 2 | 0.16 | 0.01 | 0.16 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD11 | 2 | 0.15 | 0.01 | 0.15 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD12 | 2 | 0.15 | 0.01 | 0.15 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD13 | 2 | 0.15 | 0.01 | 0.15 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD21 | 2 | 0.15 | 0.01 | 0.15 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD22 | 2 | 0.15 | 0.01 | 0.15 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD23 | 2 | 0.15 | 0.01 | 0.15 |
| (1,1606) | 1:A:128:GLN:H | 1:A:133:TYR:HD1 | 2 | 0.15 | 0.01 | 0.15 |
| (1,1606) | 1:A:128:GLN:H | 1:A:133:TYR:HD2 | 2 | 0.15 | 0.01 | 0.15 |
| (1,2994) | 1:B:126:GLU:HB2 | 1:B:133:TYR:HB3 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2994) | 1:B:126:GLU:HB3 | 1:B:133:TYR:HB3 | 2 | 0.15 | 0.02 | 0.15 |
| (1,4278) | 1:B:169:MET:H | 1:B:169:MET:HA | 2 | 0.15 | 0.01 | 0.15 |
| (1,1260) | 1:A:166:GLU:HG3 | 1:A:168:PRO:HD2 | 2 | 0.15 | 0.04 | 0.15 |
| (1,1260) | 1:A:166:GLU:HG2 | 1:A:168:PRO:HD2 | 2 | 0.15 | 0.04 | 0.15 |
| (1,1260) | 1:A:166:GLU:HG2 | 1:A:168:PRO:HD3 | 2 | 0.15 | 0.04 | 0.15 |
| (1,1260) | 1:A:166:GLU:HG3 | 1:A:168:PRO:HD3 | 2 | 0.15 | 0.04 | 0.15 |
| (1,1745) | 1:A:148:VAL:H | 1:A:146:PRO:HD2 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1745) | 1:A:148:VAL:H | 1:A:146:PRO:HD3 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB1 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB2 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB3 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1958) | 1:A:165:VAL:H | 1:A:166:GLU:HB3 | 2 | 0.15 | 0.04 | 0.15 |
| (1,3903) | 1:B:129:ASP:H | 1:B:129:ASP:HB3 | 2 | 0.15 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,29) | 1:A:94:ARG:HA | 1:A:168:PRO:HA | 2 | 0.15 | 0.03 | 0.15 |
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD21 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD22 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD23 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3453) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB2 | 2 | 0.15 | 0.0 | 0.15 |
| (1,3453) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB2 | 2 | 0.15 | 0.0 | 0.15 |
| (1,3453) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB2 | 2 | 0.15 | 0.0 | 0.15 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG21 | 2 | 0.14 | 0.03 | 0.14 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG23 | 2 | 0.14 | 0.03 | 0.14 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG21 | 2 | 0.14 | 0.03 | 0.14 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG23 | 2 | 0.14 | 0.03 | 0.14 |
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG21 | 2 | 0.14 | 0.03 | 0.14 |
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG23 | 2 | 0.14 | 0.03 | 0.14 |
| (1,71) | 1:A:95:TRP:HB2 | 1:A:168:PRO:HB2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,71) | 1:A:95:TRP:HB3 | 1:A:168:PRO:HB2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,764) | 1:A:129:ASP:HA | 1:A:129:ASP:HB3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1382) | 1:A:102:ASN:HD22 | 1:A:161:GLY:HA2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,2304) | 1:B:94:ARG:HA | 1:B:94:ARG:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2883) | 1:B:119:GLU:HA | 1:B:119:GLU:HG3 | 2 | 0.14 | 0.0 | 0.14 |
| (1,3479) | 1:B:159:PRO:HA | 1:B:159:PRO:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,3608) | 1:B:94:ARG:H | 1:B:169:MET:HG2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,60) | 1:A:95:TRP:HB2 | 1:A:95:TRP:HE3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1174) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HG | 2 | 0.14 | 0.01 | 0.14 |
| (1,1174) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HG | 2 | 0.14 | 0.01 | 0.14 |
| (1,1174) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HG | 2 | 0.14 | 0.01 | 0.14 |
| (1,1668) | 1:A:135:SER:H | 1:A:135:SER:HB3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG21 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG23 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2357) | 1:B:95:TRP:HE3 | 1:B:166:GLU:HA | 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) |
|---|---|---|---|---|---|---|
| (1,2752) | 1:B:112:LYS:HD2 | 1:B:114:LYS:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,2752) | 1:B:112:LYS:HD3 | 1:B:114:LYS:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,3498) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG21 | 2 | 0.14 | 0.01 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG23 | 2 | 0.14 | 0.01 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,117) | 1:A:96:ARG:HD2 | 1:A:166:GLU:HG2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,117) | 1:A:96:ARG:HD3 | 1:A:166:GLU:HG3 | 2 | 0.13 | 0.01 | 0.13 |
| (1,117) | 1:A:96:ARG:HD3 | 1:A:166:GLU:HG2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,117) | 1:A:96:ARG:HD2 | 1:A:166:GLU:HG3 | 2 | 0.13 | 0.01 | 0.13 |
| (1,812) | 1:A:136:ARG:HA | 1:A:136:ARG:HD2 | 2 | 0.13 | 0.0 | 0.13 |
| (1,852) | 1:A:141:LYS:HG2 | 1:A:141:LYS:HE2 | 2 | 0.13 | 0.0 | 0.13 |
| (1,1428) | 1:A:109:LEU:H | 1:A:109:LEU:HB3 | 2 | 0.13 | 0.01 | 0.13 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG21 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG22 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG23 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG11 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG12 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG13 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1543) | 1:A:120:ILE:H | 1:A:140:ARG:HB2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,1543) | 1:A:120:ILE:H | 1:A:140:ARG:HB3 | 2 | 0.13 | 0.01 | 0.13 |
| (1,1546) | 1:A:120:ILE:H | 1:A:142:TYR:H | 2 | 0.13 | 0.02 | 0.13 |
| (1,1600) | 1:A:128:GLN:H | 1:A:127:ARG:HD2 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1622) | 1:A:129:ASP:H | 1:A:129:ASP:HB3 | 2 | 0.13 | 0.02 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG21 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG22 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG23 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG21 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG22 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG23 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG21 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG22 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG23 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG21 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG22 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG23 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG21 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG22 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG23 | 2 | 0.13 | 0.0 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG21 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG22 | 2 | 0.13 | 0.0 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG23 | 2 | 0.13 | 0.0 | 0.13 |
| (1,3266) | 1:B:148:VAL:HA | 1:B:149:ASP:HB3 | 2 | 0.13 | 0.02 | 0.13 |
| (1,4239) | 1:B:165:VAL:H | 1:B:166:GLU:HB3 | 2 | 0.13 | 0.01 | 0.13 |
| (1,604) | 1:A:119:GLU:HA | 1:A:120:ILE:HG12 | 2 | 0.12 | 0.02 | 0.12 |
| (1,608) | 1:A:119:GLU:HA | 1:A:141:LYS:HA | 2 | 0.12 | 0.01 | 0.12 |
| (1,713) | 1:A:126:GLU:HB2 | 1:A:133:TYR:HB3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,713) | 1:A:126:GLU:HB3 | 1:A:133:TYR:HB3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1762) | 1:A:149:ASP:H | 1:A:152:GLN:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD11 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD12 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD13 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD21 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD22 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD23 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG11 | 1:B:142:TYR:HD1 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG11 | 1:B:142:TYR:HD2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG12 | 1:B:142:TYR:HD1 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG12 | 1:B:142:TYR:HD2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG13 | 1:B:142:TYR:HD1 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG13 | 1:B:142:TYR:HD2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3879) | 1:B:128:GLN:H | 1:B:127:ARG:HG2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD11 | 2 | 0.12 | 0.01 | 0.12 |
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD12 | 2 | 0.12 | 0.01 | 0.12 |
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD13 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2382) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HA | 2 | 0.12 | 0.01 | 0.12 |
| (1,2885) | 1:B:119:GLU:HA | 1:B:120:ILE:HG12 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2933) | 1:B:120:ILE:HD11 | 1:B:140:ARG:HB2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2933) | 1:B:120:ILE:HD12 | 1:B:140:ARG:HB2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2933) | 1:B:120:ILE:HD13 | 1:B:140:ARG:HB2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,4135) | 1:B:155:SER:H | 1:B:166:GLU:HG2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,4135) | 1:B:155:SER:H | 1:B:166:GLU:HG3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,719) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HD1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,719) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HD2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1950) | 1:A:165:VAL:H | 1:A:96:ARG:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1950) | 1:A:165:VAL:H | 1:A:96:ARG:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2023) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2023) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD2 | 2 | 0.12 | 0.0 | 0.12 |

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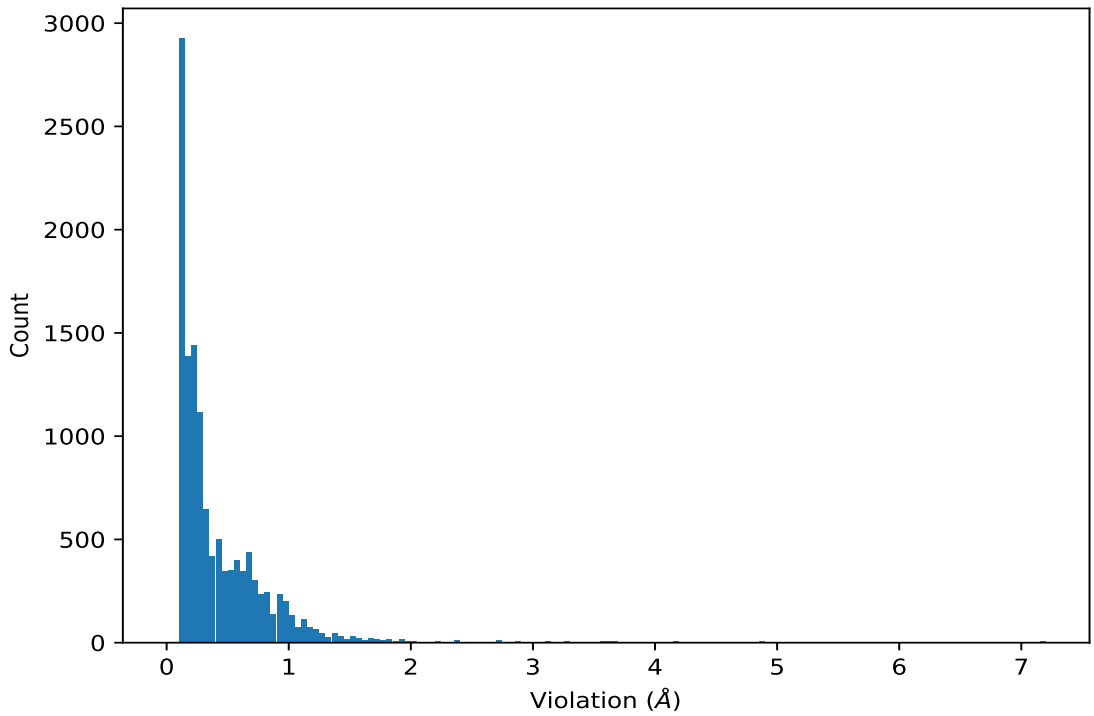
| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,2155) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2155) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,2291) | 1:B:91:THR:HA | 1:B:91:THR:HB | 2 | 0.12 | 0.0 | 0.12 |
| (1,3723) | 1:B:110:THR:H | 1:B:122:GLY:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD11 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD12 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD13 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD23 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD23 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD23 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD23 | 2 | 0.11 | 0.0 | 0.11 |

[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) |
|---|---|---|---|---|
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 5 | 7.17 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 5 | 7.17 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 5 | 7.17 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 4 | 7.16 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 4 | 7.16 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 4 | 7.16 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 5 | 6.54 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 8 | 6.54 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 9 | 6.42 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 3 | 6.11 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 3 | 6.11 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 3 | 6.11 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 6 | 6.06 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 6 | 6.06 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 6 | 6.06 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 3 | 6.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 4 | 5.86 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 6 | 5.81 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 7 | 5.77 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 7 | 5.77 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 3 | 5.52 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 2 | 5.46 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 8 | 5.41 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 8 | 5.41 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 8 | 5.41 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 2 | 5.36 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 2 | 5.36 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 2 | 5.36 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 7 | 5.01 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 3 | 4.95 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 3 | 4.95 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 9 | 4.91 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 9 | 4.91 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 9 | 4.91 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 9 | 4.91 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 10 | 4.89 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 4 | 4.86 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 9 | 4.86 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 9 | 4.86 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 9 | 4.86 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 3 | 4.7 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 3 | 4.7 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 3 | 4.7 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB1 | 5 | 4.65 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB2 | 5 | 4.65 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB3 | 5 | 4.65 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 4 | 4.64 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 4 | 4.64 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 4 | 4.64 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 1 | 4.56 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 1 | 4.56 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 1 | 4.56 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 1 | 4.54 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 1 | 4.54 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 6 | 4.45 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 6 | 4.45 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 4 | 4.42 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 4 | 4.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 1 | 4.3 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 1 | 4.3 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 1 | 4.3 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 10 | 4.26 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 10 | 4.26 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 8 | 4.19 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 8 | 4.19 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 8 | 4.19 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 4 | 4.15 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 4 | 4.15 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 10 | 4.06 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 10 | 4.06 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 10 | 3.92 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 10 | 3.92 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 10 | 3.92 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE2 | 5 | 3.84 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE3 | 5 | 3.84 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 9 | 3.8 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 9 | 3.8 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 9 | 3.8 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE2 | 4 | 3.73 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE3 | 4 | 3.73 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 8 | 3.71 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 10 | 3.67 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 10 | 3.67 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 10 | 3.67 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 10 | 3.67 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 2 | 3.66 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 2 | 3.66 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 2 | 3.66 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 8 | 3.64 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 8 | 3.64 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 8 | 3.64 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 4 | 3.63 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 4 | 3.63 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 4 | 3.63 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 8 | 3.59 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 8 | 3.59 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 2 | 3.59 |
| (1,2) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HB3 | 5 | 3.57 |
| (1,2) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HB3 | 5 | 3.57 |
| (1,2) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HB3 | 5 | 3.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 3 | 3.54 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 3 | 3.54 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 2 | 3.52 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 2 | 3.52 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 10 | 3.46 |
| (1,2) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HB3 | 3 | 3.45 |
| (1,2) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HB3 | 3 | 3.45 |
| (1,2) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HB3 | 3 | 3.45 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 1 | 3.44 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 6 | 3.42 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 1 | 3.38 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB1 | 9 | 3.36 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB2 | 9 | 3.36 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB3 | 9 | 3.36 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 7 | 3.27 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 7 | 3.27 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 7 | 3.27 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 2 | 3.26 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 2 | 3.26 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 1 | 3.2 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 1 | 3.2 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 1 | 3.2 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 1 | 3.2 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 1 | 3.14 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 1 | 3.14 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 1 | 3.14 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 8 | 3.14 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 8 | 3.14 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB1 | 4 | 3.07 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB2 | 4 | 3.07 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB3 | 4 | 3.07 |
| (1,2283) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HB3 | 7 | 3.04 |
| (1,2283) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HB3 | 7 | 3.04 |
| (1,2283) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HB3 | 7 | 3.04 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 2 | 2.96 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 2 | 2.96 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 2 | 2.96 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 2 | 2.96 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 3 | 2.9 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 3 | 2.9 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 1 | 2.89 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 1 | 2.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE2 | 6 | 2.88 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE3 | 6 | 2.88 |
| (1,1) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HA | 5 | 2.84 |
| (1,1) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HA | 5 | 2.84 |
| (1,1) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HA | 5 | 2.84 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 6 | 2.79 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 6 | 2.79 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB1 | 6 | 2.74 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB2 | 6 | 2.74 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB3 | 6 | 2.74 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 4 | 2.74 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 4 | 2.74 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 4 | 2.74 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 4 | 2.74 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG21 | 3 | 2.7 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG22 | 3 | 2.7 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG23 | 3 | 2.7 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 4 | 2.64 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 8 | 2.64 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG21 | 5 | 2.56 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG22 | 5 | 2.56 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG23 | 5 | 2.56 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 2 | 2.52 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 2 | 2.52 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 5 | 2.47 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 1 | 2.42 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 1 | 2.42 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 7 | 2.41 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 6 | 2.37 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 6 | 2.37 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 6 | 2.37 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 6 | 2.37 |
| (1,2283) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HB3 | 10 | 2.36 |
| (1,2283) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HB3 | 10 | 2.36 |
| (1,2283) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HB3 | 10 | 2.36 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 8 | 2.35 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 8 | 2.35 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 10 | 2.35 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 10 | 2.35 |
| (1,2011) | 1:A:172:LEU:H | 1:A:145:PRO:HA | 1 | 2.28 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 9 | 2.25 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 9 | 2.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 6 | 2.23 |
| (1,2) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HB3 | 7 | 2.23 |
| (1,2) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HB3 | 7 | 2.23 |
| (1,2) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HB3 | 7 | 2.23 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 4 | 2.2 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 4 | 2.2 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 4 | 2.2 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 4 | 2.2 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 7 | 2.15 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 7 | 2.15 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 7 | 2.15 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 7 | 2.15 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG21 | 3 | 2.14 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG22 | 3 | 2.14 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG23 | 3 | 2.14 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 9 | 2.13 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 10 | 2.07 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 10 | 2.07 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 10 | 2.07 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB1 | 8 | 2.01 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB2 | 8 | 2.01 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB3 | 8 | 2.01 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD1 | 4 | 2.01 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD2 | 4 | 2.01 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 4 | 2.0 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 4 | 2.0 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 3 | 1.99 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 3 | 1.99 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 3 | 1.99 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 3 | 1.99 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 10 | 1.99 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 4 | 1.98 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 4 | 1.98 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 4 | 1.98 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 4 | 1.95 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 4 | 1.95 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 4 | 1.95 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD2 | 5 | 1.94 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD3 | 5 | 1.94 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB1 | 1 | 1.94 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB2 | 1 | 1.94 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB3 | 1 | 1.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 1 | 1.94 |
| (1,2283) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HB3 | 5 | 1.93 |
| (1,2283) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HB3 | 5 | 1.93 |
| (1,2283) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HB3 | 5 | 1.93 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD2 | 9 | 1.93 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD3 | 9 | 1.93 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB1 | 1 | 1.91 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB2 | 1 | 1.91 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB3 | 1 | 1.91 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 5 | 1.87 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 5 | 1.87 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 5 | 1.87 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 1 | 1.87 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 1 | 1.87 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 5 | 1.85 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 5 | 1.85 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 5 | 1.85 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 8 | 1.84 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 7 | 1.84 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 7 | 1.84 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 7 | 1.84 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 8 | 1.84 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 1 | 1.83 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB1 | 10 | 1.83 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB2 | 10 | 1.83 |
| (1,1987) | 1:A:169:MET:H | 1:A:92:ALA:HB3 | 10 | 1.83 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 8 | 1.83 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 7 | 1.8 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 7 | 1.8 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 7 | 1.8 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 1 | 1.8 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 3 | 1.8 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 8 | 1.79 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 8 | 1.79 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 9 | 1.79 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 9 | 1.79 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 8 | 1.78 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 7 | 1.77 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 7 | 1.77 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 7 | 1.75 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 7 | 1.75 |
| (1,2284) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB2 | 8 | 1.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2284) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB2 | 8 | 1.75 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 6 | 1.74 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 6 | 1.74 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 6 | 1.74 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 10 | 1.74 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD2 | 10 | 1.74 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD3 | 10 | 1.74 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 8 | 1.73 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 8 | 1.73 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 8 | 1.73 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 8 | 1.73 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 2 | 1.73 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 2 | 1.73 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB1 | 7 | 1.73 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB2 | 7 | 1.73 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB3 | 7 | 1.73 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 10 | 1.7 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 2 | 1.69 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 2 | 1.69 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 2 | 1.69 |
| (1,1) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HA | 3 | 1.69 |
| (1,1) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HA | 3 | 1.69 |
| (1,1) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HA | 3 | 1.69 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 3 | 1.68 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 4 | 1.68 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 2 | 1.68 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 2 | 1.68 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 2 | 1.68 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG2 | 5 | 1.68 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG3 | 5 | 1.68 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 2 | 1.67 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 10 | 1.67 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE2 | 7 | 1.67 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE3 | 7 | 1.67 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 7 | 1.66 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 1 | 1.66 |
| (1,2302) | 1:B:93:ASP:HB3 | 1:B:94:ARG:HG2 | 7 | 1.65 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 3 | 1.65 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 7 | 1.64 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 5 | 1.64 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 4 | 1.63 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 4 | 1.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 6 | 1.63 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 3 | 1.61 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 3 | 1.61 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 3 | 1.61 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 4 | 1.61 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 7 | 1.6 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 3 | 1.6 |
| (1,3601) | 1:B:94:ARG:H | 1:B:92:ALA:HA | 7 | 1.59 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 3 | 1.59 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 6 | 1.59 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 6 | 1.59 |
| (1,4292) | 1:B:172:LEU:H | 1:B:145:PRO:HA | 5 | 1.58 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 8 | 1.58 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 10 | 1.58 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 9 | 1.58 |
| (1,2283) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HB3 | 1 | 1.58 |
| (1,2283) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HB3 | 1 | 1.58 |
| (1,2283) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HB3 | 1 | 1.58 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 10 | 1.57 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 10 | 1.57 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 7 | 1.57 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 5 | 1.57 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 5 | 1.56 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 10 | 1.55 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 10 | 1.55 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 10 | 1.55 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 5 | 1.55 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 1 | 1.55 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 2 | 1.55 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 6 | 1.54 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 4 | 1.54 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD2 | 5 | 1.54 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD3 | 5 | 1.54 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD2 | 6 | 1.54 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD3 | 6 | 1.54 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 2 | 1.54 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 4 | 1.54 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD1 | 9 | 1.53 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD2 | 9 | 1.53 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 4 | 1.53 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 7 | 1.53 |
| (1,2157) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 8 | 1.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2025) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 8 | 1.53 |
| (1,841) | 1:A:140:ARG:HG2 | 1:A:142:TYR:HE1 | 3 | 1.52 |
| (1,841) | 1:A:140:ARG:HG2 | 1:A:142:TYR:HE2 | 3 | 1.52 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 7 | 1.52 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 4 | 1.52 |
| (1,1320) | 1:A:94:ARG:H | 1:A:92:ALA:HA | 1 | 1.52 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 2 | 1.52 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD1 | 7 | 1.51 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD2 | 7 | 1.51 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG3 | 8 | 1.51 |
| (1,3582) | 1:B:169:MET:HB3 | 1:B:171:LYS:HG2 | 8 | 1.51 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 9 | 1.5 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 9 | 1.5 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 4 | 1.5 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 4 | 1.5 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 6 | 1.5 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 10 | 1.5 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD22 | 3 | 1.5 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD21 | 3 | 1.5 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 1 | 1.49 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 10 | 1.49 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 6 | 1.49 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 9 | 1.49 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 9 | 1.48 |
| (1,2004) | 1:A:171:LYS:H | 1:A:169:MET:HA | 10 | 1.48 |
| (1,1654) | 1:A:134:ILE:H | 1:A:127:ARG:HB2 | 1 | 1.48 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 1 | 1.48 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 5 | 1.47 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 5 | 1.47 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 5 | 1.47 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 2 | 1.47 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 2 | 1.47 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 2 | 1.46 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 3 | 1.46 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 5 | 1.45 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 9 | 1.45 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 6 | 1.45 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 8 | 1.44 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 8 | 1.44 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 7 | 1.44 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 7 | 1.44 |
| (1,286) | 1:A:105:ALA:HA | 1:A:108:GLU:HB2 | 9 | 1.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE2 | 9 | 1.44 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE3 | 9 | 1.44 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 5 | 1.44 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 5 | 1.44 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 5 | 1.44 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 5 | 1.44 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 7 | 1.43 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 7 | 1.43 |
| (1,16) | 1:A:93:ASP:HA | 1:A:94:ARG:HD2 | 5 | 1.43 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 3 | 1.41 |
| (1,2152) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2152) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2152) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2152) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2152) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2152) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2020) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2020) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2020) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2020) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2020) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,2020) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 1 | 1.41 |
| (1,1766) | 1:A:149:ASP:H | 1:A:169:MET:HG3 | 10 | 1.41 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 7 | 1.41 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB1 | 5 | 1.4 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB2 | 5 | 1.4 |
| (1,4284) | 1:B:171:LYS:H | 1:B:92:ALA:HB3 | 5 | 1.4 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 5 | 1.4 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 9 | 1.4 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 9 | 1.4 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 4 | 1.4 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 4 | 1.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 5 | 1.4 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 9 | 1.39 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 6 | 1.39 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 6 | 1.39 |
| (1,3005) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB3 | 4 | 1.38 |
| (1,2) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HB3 | 6 | 1.38 |
| (1,2) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HB3 | 6 | 1.38 |
| (1,2) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HB3 | 6 | 1.38 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE1 | 8 | 1.37 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE2 | 8 | 1.37 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG21 | 6 | 1.37 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG22 | 6 | 1.37 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG23 | 6 | 1.37 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG21 | 10 | 1.37 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG22 | 10 | 1.37 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG23 | 10 | 1.37 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 1 | 1.37 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 1 | 1.37 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 1 | 1.37 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 7 | 1.36 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 10 | 1.36 |
| (1,1766) | 1:A:149:ASP:H | 1:A:169:MET:HG3 | 5 | 1.36 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 9 | 1.35 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 6 | 1.35 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 6 | 1.35 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 9 | 1.35 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 9 | 1.35 |
| (1,2290) | 1:B:90:HIS:HB3 | 1:B:91:THR:HA | 7 | 1.35 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB2 | 6 | 1.35 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB3 | 6 | 1.35 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 1 | 1.34 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 1 | 1.34 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 1 | 1.34 |
| (1,2327) | 1:B:94:ARG:HG3 | 1:B:168:PRO:HA | 7 | 1.34 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 8 | 1.34 |
| (1,110) | 1:A:96:ARG:HG3 | 1:A:166:GLU:HB3 | 10 | 1.34 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 9 | 1.33 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 6 | 1.33 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 6 | 1.33 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 3 | 1.33 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 2 | 1.32 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 2 | 1.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 9 | 1.32 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 9 | 1.32 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 9 | 1.32 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 6 | 1.32 |
| (1,4285) | 1:B:171:LYS:H | 1:B:169:MET:HA | 5 | 1.31 |
| (1,2302) | 1:B:93:ASP:HB3 | 1:B:94:ARG:HG2 | 3 | 1.31 |
| (1,2282) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HA | 7 | 1.31 |
| (1,2282) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HA | 7 | 1.31 |
| (1,2282) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HA | 7 | 1.31 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 3 | 1.3 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 3 | 1.3 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 1 | 1.3 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 1 | 1.3 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 1 | 1.3 |
| (1,2193) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 2 | 1.3 |
| (1,2061) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 2 | 1.3 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 3 | 1.3 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 5 | 1.29 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 5 | 1.29 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 5 | 1.29 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 1 | 1.29 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 1 | 1.29 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 1 | 1.29 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 3 | 1.28 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 3 | 1.28 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 1 | 1.28 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 2 | 1.28 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 7 | 1.28 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 5 | 1.27 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 9 | 1.27 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 3 | 1.27 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 3 | 1.27 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 2 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 2 | 1.27 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 5 | 1.27 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 9 | 1.27 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD1 | 1 | 1.27 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD2 | 1 | 1.27 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 4 | 1.26 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 8 | 1.26 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 3 | 1.26 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD1 | 3 | 1.26 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD2 | 3 | 1.26 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 1 | 1.26 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 2 | 1.25 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 4 | 1.25 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 4 | 1.25 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 9 | 1.25 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 3 | 1.25 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 8 | 1.25 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD1 | 7 | 1.25 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD2 | 7 | 1.25 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 1 | 1.24 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 1 | 1.24 |
| (1,724) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB3 | 7 | 1.24 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 7 | 1.24 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 5 | 1.24 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 10 | 1.24 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 10 | 1.24 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 10 | 1.24 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 10 | 1.24 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE1 | 10 | 1.23 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE2 | 10 | 1.23 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 6 | 1.23 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 9 | 1.23 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB2 | 3 | 1.23 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB3 | 3 | 1.23 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 2 | 1.23 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 9 | 1.23 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 9 | 1.23 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 9 | 1.23 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 9 | 1.23 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 7 | 1.22 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 7 | 1.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 7 | 1.22 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 2 | 1.22 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 2 | 1.22 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG2 | 4 | 1.22 |
| (1,2016) | 1:A:174:THR:H | 1:A:171:LYS:HG3 | 4 | 1.22 |
| (1,4267) | 1:B:167:ALA:H | 1:B:169:MET:H | 2 | 1.21 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 6 | 1.21 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 6 | 1.21 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 6 | 1.21 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD22 | 9 | 1.21 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD21 | 9 | 1.21 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 3 | 1.21 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 3 | 1.21 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 6 | 1.21 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 10 | 1.21 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 10 | 1.21 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 10 | 1.21 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 1 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD11 | 4 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD12 | 4 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD13 | 4 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD21 | 4 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD22 | 4 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD23 | 4 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD11 | 5 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD12 | 5 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD13 | 5 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD21 | 5 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD22 | 5 | 1.21 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD23 | 5 | 1.21 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 6 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 4 | 1.21 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 4 | 1.21 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 4 | 1.21 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 8 | 1.2 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 8 | 1.2 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 2 | 1.2 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE1 | 1 | 1.2 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE2 | 1 | 1.2 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 10 | 1.2 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 10 | 1.2 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 2 | 1.2 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 3 | 1.2 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 5 | 1.2 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 2 | 1.2 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 2 | 1.2 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 2 | 1.2 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 2 | 1.2 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 2 | 1.2 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 9 | 1.2 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 8 | 1.2 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 8 | 1.2 |
| (1,2193) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 7 | 1.2 |
| (1,2061) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 7 | 1.2 |
| (1,2004) | 1:A:171:LYS:H | 1:A:169:MET:HA | 9 | 1.2 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 5 | 1.19 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 2 | 1.19 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 2 | 1.19 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 8 | 1.19 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 8 | 1.19 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 8 | 1.19 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 4 | 1.19 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 4 | 1.19 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 6 | 1.19 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 7 | 1.19 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 8 | 1.19 |
| (1,2157) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 2 | 1.19 |
| (1,2025) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 2 | 1.19 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 6 | 1.19 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 6 | 1.19 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 6 | 1.19 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 2 | 1.18 |
| (1,724) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB3 | 9 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 9 | 1.18 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD22 | 1 | 1.18 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD21 | 1 | 1.18 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 3 | 1.17 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 3 | 1.17 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 3 | 1.17 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 1 | 1.17 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 1 | 1.17 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 1 | 1.17 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 5 | 1.17 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 5 | 1.17 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 5 | 1.17 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 5 | 1.17 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 5 | 1.17 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 5 | 1.17 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 1 | 1.17 |
| (1,2282) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HA | 2 | 1.17 |
| (1,2282) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HA | 2 | 1.17 |
| (1,2282) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HA | 2 | 1.17 |
| (1,839) | 1:A:140:ARG:HB2 | 1:A:140:ARG:HD2 | 6 | 1.16 |
| (1,839) | 1:A:140:ARG:HB3 | 1:A:140:ARG:HD2 | 6 | 1.16 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 9 | 1.16 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 4 | 1.16 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 4 | 1.16 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 6 | 1.16 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 6 | 1.16 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 6 | 1.16 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 2 | 1.16 |
| (1,2391) | 1:B:96:ARG:HG3 | 1:B:166:GLU:HB3 | 6 | 1.16 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 7 | 1.16 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD22 | 1 | 1.16 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD21 | 1 | 1.16 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 7 | 1.16 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 7 | 1.16 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 7 | 1.16 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 5 | 1.15 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 5 | 1.15 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 5 | 1.15 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 5 | 1.15 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 10 | 1.15 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 10 | 1.15 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 4 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 4 | 1.15 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 4 | 1.15 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 3 | 1.15 |
| (1,2193) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 9 | 1.15 |
| (1,2061) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 9 | 1.15 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD22 | 5 | 1.15 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD21 | 5 | 1.15 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 2 | 1.15 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 2 | 1.15 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 2 | 1.15 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 3 | 1.14 |
| (1,44) | 1:A:94:ARG:HG2 | 1:A:166:GLU:HB2 | 8 | 1.14 |
| (1,44) | 1:A:94:ARG:HG3 | 1:A:166:GLU:HB2 | 8 | 1.14 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 1 | 1.14 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 1 | 1.14 |
| (1,2193) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 1 | 1.14 |
| (1,2061) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 1 | 1.14 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 10 | 1.14 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 10 | 1.14 |
| (1,1614) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB2 | 7 | 1.14 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 9 | 1.14 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 5 | 1.13 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 8 | 1.13 |
| (1,3566) | 1:B:168:PRO:HD2 | 1:B:169:MET:HA | 6 | 1.13 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 9 | 1.13 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 9 | 1.13 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 9 | 1.13 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 3 | 1.13 |
| (1,2300) | 1:B:93:ASP:HB2 | 1:B:94:ARG:HG2 | 7 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD11 | 6 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD12 | 6 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD13 | 6 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD21 | 6 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD22 | 6 | 1.13 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD23 | 6 | 1.13 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB1 | 3 | 1.13 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB2 | 3 | 1.13 |
| (1,2003) | 1:A:171:LYS:H | 1:A:92:ALA:HB3 | 3 | 1.13 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 3 | 1.13 |
| (1,710) | 1:A:126:GLU:HA | 1:A:135:SER:HB2 | 2 | 1.12 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 4 | 1.12 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 6 | 1.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 9 | 1.12 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 9 | 1.12 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 9 | 1.12 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 8 | 1.12 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 7 | 1.12 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 4 | 1.12 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 4 | 1.12 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 4 | 1.12 |
| (1,2194) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 3 | 1.12 |
| (1,2157) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 4 | 1.12 |
| (1,2062) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 3 | 1.12 |
| (1,2025) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 4 | 1.12 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 8 | 1.12 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 8 | 1.12 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 8 | 1.12 |
| (1,990) | 1:A:148:VAL:HA | 1:A:169:MET:HB2 | 3 | 1.11 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 10 | 1.11 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 10 | 1.11 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD1 | 10 | 1.11 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD2 | 10 | 1.11 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 9 | 1.11 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 9 | 1.11 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 9 | 1.11 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 10 | 1.11 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 10 | 1.11 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE1 | 3 | 1.11 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE2 | 3 | 1.11 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE1 | 3 | 1.11 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE2 | 3 | 1.11 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE1 | 3 | 1.11 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE2 | 3 | 1.11 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 3 | 1.11 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 9 | 1.11 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 9 | 1.11 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 9 | 1.11 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 9 | 1.11 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 3 | 1.11 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 3 | 1.11 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 3 | 1.11 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 5 | 1.11 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 5 | 1.11 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 5 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE1 | 1 | 1.1 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE2 | 1 | 1.1 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 8 | 1.1 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 9 | 1.1 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG11 | 10 | 1.1 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG12 | 10 | 1.1 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG13 | 10 | 1.1 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 9 | 1.1 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 2 | 1.1 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 2 | 1.1 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 2 | 1.1 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 2 | 1.1 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 2 | 1.1 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 2 | 1.1 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 5 | 1.1 |
| (1,2) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HB3 | 2 | 1.1 |
| (1,2) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HB3 | 2 | 1.1 |
| (1,2) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HB3 | 2 | 1.1 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 9 | 1.1 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 6 | 1.1 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 6 | 1.1 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 6 | 1.1 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 7 | 1.09 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 8 | 1.09 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 7 | 1.09 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 3 | 1.09 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 6 | 1.09 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 6 | 1.09 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 6 | 1.09 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 4 | 1.09 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 6 | 1.09 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 5 | 1.09 |
| (1,1269) | 1:A:167:ALA:HB1 | 1:A:168:PRO:HD2 | 9 | 1.09 |
| (1,1269) | 1:A:167:ALA:HB2 | 1:A:168:PRO:HD2 | 9 | 1.09 |
| (1,1269) | 1:A:167:ALA:HB3 | 1:A:168:PRO:HD2 | 9 | 1.09 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 8 | 1.09 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 8 | 1.09 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 8 | 1.09 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 10 | 1.09 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 1 | 1.08 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 9 | 1.08 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 9 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 9 | 1.08 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 5 | 1.08 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 7 | 1.08 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 7 | 1.08 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 7 | 1.08 |
| (1,3346) | 1:B:152:GLN:HB2 | 1:B:169:MET:HA | 6 | 1.08 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 5 | 1.08 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 5 | 1.08 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 7 | 1.08 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 8 | 1.08 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 2 | 1.08 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 3 | 1.07 |
| (1,4267) | 1:B:167:ALA:H | 1:B:169:MET:H | 9 | 1.07 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 4 | 1.07 |
| (1,3566) | 1:B:168:PRO:HD2 | 1:B:169:MET:HA | 4 | 1.07 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 1 | 1.07 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 10 | 1.07 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 9 | 1.07 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG3 | 6 | 1.07 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG2 | 6 | 1.07 |
| (1,990) | 1:A:148:VAL:HA | 1:A:169:MET:HB2 | 4 | 1.06 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 3 | 1.06 |
| (1,918) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA3 | 8 | 1.06 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 9 | 1.06 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 4 | 1.06 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 4 | 1.06 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 4 | 1.06 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 5 | 1.06 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 5 | 1.06 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 5 | 1.06 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 2 | 1.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 2 | 1.06 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 2 | 1.06 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 2 | 1.06 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 8 | 1.06 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 1 | 1.06 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 2 | 1.06 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG21 | 8 | 1.06 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG22 | 8 | 1.06 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG23 | 8 | 1.06 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE1 | 4 | 1.05 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE2 | 4 | 1.05 |
| (1,722) | 1:A:126:GLU:HG2 | 1:A:135:SER:HA | 7 | 1.05 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 8 | 1.05 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 7 | 1.05 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE1 | 3 | 1.04 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE2 | 3 | 1.04 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 5 | 1.04 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 5 | 1.04 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 5 | 1.04 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 5 | 1.04 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 6 | 1.04 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 6 | 1.04 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 6 | 1.04 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 8 | 1.04 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 8 | 1.04 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 7 | 1.04 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB1 | 8 | 1.04 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB2 | 8 | 1.04 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB3 | 8 | 1.04 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB1 | 1 | 1.04 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB2 | 1 | 1.04 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB3 | 1 | 1.04 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 9 | 1.04 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 9 | 1.04 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 4 | 1.04 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 1 | 1.04 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 1 | 1.04 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 1 | 1.04 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 1 | 1.04 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 8 | 1.04 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 8 | 1.04 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 8 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,7) | 1:A:90:HIS:HB2 | 1:A:91:THR:HA | 9 | 1.03 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB1 | 1 | 1.03 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB2 | 1 | 1.03 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB3 | 1 | 1.03 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 6 | 1.03 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 6 | 1.03 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 1 | 1.03 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 1 | 1.03 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 1 | 1.03 |
| (1,3557) | 1:B:168:PRO:HA | 1:B:169:MET:HG2 | 7 | 1.03 |
| (1,3199) | 1:B:144:LEU:HB3 | 1:B:147:GLY:HA3 | 9 | 1.03 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 2 | 1.03 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 2 | 1.03 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 2 | 1.03 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 5 | 1.03 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 5 | 1.03 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 5 | 1.03 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 5 | 1.03 |
| (1,16) | 1:A:93:ASP:HA | 1:A:94:ARG:HD2 | 8 | 1.03 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG3 | 4 | 1.03 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG2 | 4 | 1.03 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 2 | 1.03 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 2 | 1.03 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 2 | 1.03 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 7 | 1.02 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 7 | 1.02 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE1 | 6 | 1.02 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE2 | 6 | 1.02 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 1 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 4 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 4 | 1.02 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 4 | 1.02 |
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 2 | 1.02 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 2 | 1.02 |
| (1,2284) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB2 | 2 | 1.02 |
| (1,2284) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB2 | 2 | 1.02 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 7 | 1.02 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 7 | 1.02 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 7 | 1.02 |
| (1,1766) | 1:A:149:ASP:H | 1:A:169:MET:HG3 | 2 | 1.02 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 5 | 1.02 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 5 | 1.02 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 5 | 1.02 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 10 | 1.02 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 10 | 1.02 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 10 | 1.02 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 4 | 1.02 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 4 | 1.02 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 4 | 1.02 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 7 | 1.01 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 4 | 1.01 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 8 | 1.01 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 8 | 1.01 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 8 | 1.01 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 9 | 1.01 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 9 | 1.01 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 1 | 1.01 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 1 | 1.01 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 5 | 1.01 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 1 | 1.01 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE1 | 5 | 1.01 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE2 | 5 | 1.01 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE1 | 5 | 1.01 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE2 | 5 | 1.01 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE1 | 5 | 1.01 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE2 | 5 | 1.01 |
| (1,2318) | 1:B:94:ARG:HB2 | 1:B:96:ARG:HA | 7 | 1.01 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG21 | 5 | 1.01 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG22 | 5 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG23 | 5 | 1.01 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 10 | 1.0 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 10 | 1.0 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 2 | 1.0 |
| (1,3558) | 1:B:168:PRO:HA | 1:B:169:MET:HG3 | 7 | 1.0 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 1 | 1.0 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 1 | 1.0 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 1 | 1.0 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 8 | 1.0 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 7 | 1.0 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 7 | 1.0 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 7 | 1.0 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 1 | 1.0 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 1 | 1.0 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 1 | 1.0 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 1 | 1.0 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 1 | 1.0 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 1 | 1.0 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 6 | 1.0 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 6 | 1.0 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 6 | 1.0 |
| (1,2193) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 8 | 1.0 |
| (1,2061) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 8 | 1.0 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE1 | 10 | 0.99 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE2 | 10 | 0.99 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 4 | 0.99 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB1 | 4 | 0.99 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB2 | 4 | 0.99 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB3 | 4 | 0.99 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 10 | 0.99 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 9 | 0.99 |
| (1,3566) | 1:B:168:PRO:HD2 | 1:B:169:MET:HA | 5 | 0.99 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 9 | 0.99 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 9 | 0.99 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 9 | 0.99 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 3 | 0.99 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 3 | 0.99 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 3 | 0.99 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG21 | 6 | 0.99 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG22 | 6 | 0.99 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG23 | 6 | 0.99 |
| (1,2283) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HB3 | 4 | 0.99 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2283) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HB3 | 4 | 0.99 |
| (1,2283) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HB3 | 4 | 0.99 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 1 | 0.99 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 1 | 0.99 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 1 | 0.99 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 7 | 0.99 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 7 | 0.99 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 7 | 0.99 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 8 | 0.98 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 8 | 0.98 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 8 | 0.98 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB1 | 9 | 0.98 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB2 | 9 | 0.98 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB3 | 9 | 0.98 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 5 | 0.98 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 5 | 0.98 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 8 | 0.98 |
| (1,3271) | 1:B:148:VAL:HA | 1:B:169:MET:HB2 | 5 | 0.98 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 3 | 0.98 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE1 | 2 | 0.98 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE2 | 2 | 0.98 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE1 | 2 | 0.98 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE2 | 2 | 0.98 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE1 | 2 | 0.98 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE2 | 2 | 0.98 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 10 | 0.98 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 10 | 0.98 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 10 | 0.98 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 7 | 0.98 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 7 | 0.98 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 7 | 0.98 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 7 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 3 | 0.98 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD1 | 8 | 0.98 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD2 | 8 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 6 | 0.98 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 6 | 0.98 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 8 | 0.97 |
| (1,4293) | 1:B:172:LEU:H | 1:B:171:LYS:HA | 9 | 0.97 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 1 | 0.97 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 1 | 0.97 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 10 | 0.97 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 10 | 0.97 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 10 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 5 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 5 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 7 | 0.97 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 7 | 0.97 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 3 | 0.97 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 3 | 0.97 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 3 | 0.97 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 6 | 0.97 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 6 | 0.97 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 6 | 0.97 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 6 | 0.97 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 6 | 0.97 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE1 | 7 | 0.97 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE2 | 7 | 0.97 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE1 | 7 | 0.97 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE2 | 7 | 0.97 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE1 | 7 | 0.97 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE2 | 7 | 0.97 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 9 | 0.97 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 9 | 0.97 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 9 | 0.97 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 9 | 0.97 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 9 | 0.97 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 9 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 5 | 0.97 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 3 | 0.97 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 3 | 0.97 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 3 | 0.97 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 8 | 0.97 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 8 | 0.97 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 8 | 0.97 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 5 | 0.97 |
| (1,2012) | 1:A:172:LEU:H | 1:A:171:LYS:HA | 8 | 0.97 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 8 | 0.97 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 8 | 0.97 |
| (1,1012) | 1:A:148:VAL:HG11 | 1:A:169:MET:HB2 | 4 | 0.97 |
| (1,1012) | 1:A:148:VAL:HG12 | 1:A:169:MET:HB2 | 4 | 0.97 |
| (1,1012) | 1:A:148:VAL:HG13 | 1:A:169:MET:HB2 | 4 | 0.97 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 3 | 0.96 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 3 | 0.96 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB1 | 6 | 0.96 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB2 | 6 | 0.96 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB3 | 6 | 0.96 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 3 | 0.96 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 8 | 0.96 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 8 | 0.96 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 9 | 0.96 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 3 | 0.96 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 8 | 0.96 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 8 | 0.96 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 8 | 0.96 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 5 | 0.96 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 9 | 0.96 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 9 | 0.96 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 9 | 0.96 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 9 | 0.96 |
| (1,3550) | 1:B:167:ALA:HB1 | 1:B:168:PRO:HD2 | 3 | 0.96 |
| (1,3550) | 1:B:167:ALA:HB2 | 1:B:168:PRO:HD2 | 3 | 0.96 |
| (1,3550) | 1:B:167:ALA:HB3 | 1:B:168:PRO:HD2 | 3 | 0.96 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 8 | 0.96 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 8 | 0.96 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 8 | 0.96 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 9 | 0.96 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 9 | 0.96 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 9 | 0.96 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 9 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 9 | 0.96 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 4 | 0.96 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 4 | 0.96 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 9 | 0.96 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 10 | 0.96 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 7 | 0.96 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 7 | 0.96 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 6 | 0.96 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 6 | 0.96 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 6 | 0.96 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 1 | 0.96 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 1 | 0.96 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 1 | 0.96 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 7 | 0.96 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 7 | 0.96 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 7 | 0.96 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 1 | 0.95 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 1 | 0.95 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 2 | 0.95 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 2 | 0.95 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 7 | 0.95 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 7 | 0.95 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 10 | 0.95 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 10 | 0.95 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 2 | 0.95 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB1 | 10 | 0.95 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB2 | 10 | 0.95 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB3 | 10 | 0.95 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 1 | 0.95 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD11 | 9 | 0.95 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD12 | 9 | 0.95 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD13 | 9 | 0.95 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD21 | 9 | 0.95 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD22 | 9 | 0.95 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD23 | 9 | 0.95 |
| (1,4255) | 1:B:167:ALA:H | 1:B:95:TRP:HB3 | 8 | 0.95 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 2 | 0.95 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 2 | 0.95 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 2 | 0.95 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 2 | 0.95 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 7 | 0.95 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 10 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 3 | 0.95 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 3 | 0.95 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 3 | 0.95 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 7 | 0.95 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 7 | 0.95 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 4 | 0.95 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 8 | 0.95 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 2 | 0.95 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 2 | 0.95 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 2 | 0.95 |
| (1,1012) | 1:A:148:VAL:HG11 | 1:A:169:MET:HB2 | 3 | 0.95 |
| (1,1012) | 1:A:148:VAL:HG12 | 1:A:169:MET:HB2 | 3 | 0.95 |
| (1,1012) | 1:A:148:VAL:HG13 | 1:A:169:MET:HB2 | 3 | 0.95 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 8 | 0.94 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 8 | 0.94 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE1 | 3 | 0.94 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE2 | 3 | 0.94 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 8 | 0.94 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 8 | 0.94 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 8 | 0.94 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 3 | 0.94 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 3 | 0.94 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 6 | 0.94 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 7 | 0.94 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 4 | 0.94 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 4 | 0.94 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 4 | 0.94 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 9 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 9 | 0.94 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 9 | 0.94 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 5 | 0.94 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 5 | 0.94 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 5 | 0.94 |
| (1,990) | 1:A:148:VAL:HA | 1:A:169:MET:HB2 | 10 | 0.93 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 6 | 0.93 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 6 | 0.93 |
| (1,724) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB3 | 6 | 0.93 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 7 | 0.93 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 7 | 0.93 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 1 | 0.93 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 5 | 0.93 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 10 | 0.93 |
| (1,2322) | 1:B:94:ARG:HB3 | 1:B:167:ALA:HA | 4 | 0.93 |
| (1,2269) | 1:A:137:CYS:H | 1:A:137:CYS:HB3 | 4 | 0.93 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB2 | 4 | 0.93 |
| (1,2269) | 1:A:137:CYS:H | 1:B:137:CYS:HB3 | 4 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 8 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 10 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 10 | 0.93 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 10 | 0.93 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 4 | 0.92 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 4 | 0.92 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 5 | 0.92 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 5 | 0.92 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 1 | 0.92 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 3 | 0.92 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 1 | 0.92 |
| (1,3274) | 1:B:148:VAL:HA | 1:B:170:PRO:HG2 | 2 | 0.92 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 3 | 0.92 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 3 | 0.92 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 3 | 0.92 |
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 5 | 0.92 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 4 | 0.92 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 8 | 0.92 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 8 | 0.92 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 8 | 0.92 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG3 | 9 | 0.92 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG2 | 9 | 0.92 |
| (1,2194) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 4 | 0.92 |
| (1,2062) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 4 | 0.92 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 4 | 0.92 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 4 | 0.92 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 4 | 0.92 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 9 | 0.92 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 9 | 0.92 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 9 | 0.92 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 9 | 0.91 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 9 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 5 | 0.91 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 2 | 0.91 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 2 | 0.91 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 4 | 0.91 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 4 | 0.91 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 7 | 0.91 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 7 | 0.91 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 7 | 0.91 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 4 | 0.91 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 4 | 0.91 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 4 | 0.91 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE1 | 4 | 0.91 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE2 | 4 | 0.91 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 7 | 0.91 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 7 | 0.91 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 7 | 0.91 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 7 | 0.91 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 7 | 0.91 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 7 | 0.91 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 1 | 0.91 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 3 | 0.91 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 4 | 0.91 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 3 | 0.91 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 3 | 0.91 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 3 | 0.91 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 1 | 0.9 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 7 | 0.9 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB1 | 2 | 0.9 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB2 | 2 | 0.9 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB3 | 2 | 0.9 |
| (1,4267) | 1:B:167:ALA:H | 1:B:169:MET:H | 10 | 0.9 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 6 | 0.9 |
| (1,3303) | 1:B:148:VAL:HG21 | 1:B:170:PRO:HG2 | 2 | 0.9 |
| (1,3303) | 1:B:148:VAL:HG22 | 1:B:170:PRO:HG2 | 2 | 0.9 |
| (1,3303) | 1:B:148:VAL:HG23 | 1:B:170:PRO:HG2 | 2 | 0.9 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE1 | 8 | 0.9 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE2 | 8 | 0.9 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 7 | 0.9 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 8 | 0.9 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 8 | 0.9 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 8 | 0.9 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE1 | 10 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE2 | 10 | 0.9 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE1 | 10 | 0.9 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE2 | 10 | 0.9 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE1 | 10 | 0.9 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE2 | 10 | 0.9 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 5 | 0.9 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 3 | 0.9 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 8 | 0.9 |
| (1,1916) | 1:A:162:THR:H | 1:A:102:ASN:HB3 | 6 | 0.9 |
| (1,1916) | 1:A:162:THR:H | 1:A:102:ASN:HB3 | 9 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 4 | 0.9 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 4 | 0.9 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 8 | 0.9 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 10 | 0.89 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 7 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 7 | 0.89 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 7 | 0.89 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG11 | 4 | 0.89 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG12 | 4 | 0.89 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG13 | 4 | 0.89 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 7 | 0.89 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 7 | 0.89 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 7 | 0.89 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 10 | 0.89 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 4 | 0.89 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 2 | 0.89 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 2 | 0.89 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 2 | 0.89 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 10 | 0.89 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 10 | 0.89 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 10 | 0.89 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 1 | 0.89 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 10 | 0.89 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 10 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 2 | 0.89 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 2 | 0.89 |
| (1,839) | 1:A:140:ARG:HB2 | 1:A:140:ARG:HD2 | 7 | 0.88 |
| (1,839) | 1:A:140:ARG:HB3 | 1:A:140:ARG:HD2 | 7 | 0.88 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 7 | 0.88 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 6 | 0.88 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 4 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 6 | 0.88 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG2 | 10 | 0.88 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG3 | 10 | 0.88 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 5 | 0.88 |
| (1,1018) | 1:A:148:VAL:HG21 | 1:A:168:PRO:HD3 | 10 | 0.88 |
| (1,1018) | 1:A:148:VAL:HG22 | 1:A:168:PRO:HD3 | 10 | 0.88 |
| (1,1018) | 1:A:148:VAL:HG23 | 1:A:168:PRO:HD3 | 10 | 0.88 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 4 | 0.87 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 10 | 0.87 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 10 | 0.87 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE1 | 9 | 0.87 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE2 | 9 | 0.87 |
| (1,704) | 1:A:125:GLU:HA | 1:A:135:SER:HB3 | 3 | 0.87 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE1 | 5 | 0.87 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE2 | 5 | 0.87 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 7 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 3 | 0.87 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 3 | 0.87 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 8 | 0.87 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 4 | 0.87 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 4 | 0.87 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 4 | 0.87 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE1 | 6 | 0.87 |
| (1,254) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HE2 | 6 | 0.87 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE1 | 6 | 0.87 |
| (1,254) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HE2 | 6 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE1 | 6 | 0.87 |
| (1,254) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HE2 | 6 | 0.87 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 10 | 0.87 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 10 | 0.87 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 10 | 0.87 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 10 | 0.87 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 10 | 0.87 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 10 | 0.87 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG3 | 3 | 0.87 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG2 | 3 | 0.87 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 9 | 0.87 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 4 | 0.87 |
| (1,2004) | 1:A:171:LYS:H | 1:A:169:MET:HA | 2 | 0.87 |
| (1,2004) | 1:A:171:LYS:H | 1:A:169:MET:HA | 8 | 0.87 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 9 | 0.87 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 9 | 0.87 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 9 | 0.87 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 7 | 0.86 |
| (1,684) | 1:A:123:LYS:HA | 1:A:135:SER:HB3 | 5 | 0.86 |
| (1,3763) | 1:B:114:LYS:H | 1:B:115:ASP:HB2 | 2 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 10 | 0.86 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 10 | 0.86 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 5 | 0.86 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 5 | 0.86 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 8 | 0.86 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 8 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 9 | 0.86 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 10 | 0.86 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 4 | 0.86 |
| (1,2322) | 1:B:94:ARG:HB3 | 1:B:167:ALA:HA | 5 | 0.86 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE2 | 10 | 0.86 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE3 | 10 | 0.86 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 8 | 0.86 |
| (1,1012) | 1:A:148:VAL:HG11 | 1:A:169:MET:HB2 | 10 | 0.86 |
| (1,1012) | 1:A:148:VAL:HG12 | 1:A:169:MET:HB2 | 10 | 0.86 |
| (1,1012) | 1:A:148:VAL:HG13 | 1:A:169:MET:HB2 | 10 | 0.86 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 6 | 0.85 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 6 | 0.85 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 6 | 0.85 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 6 | 0.85 |
| (1,4293) | 1:B:172:LEU:H | 1:B:171:LYS:HA | 3 | 0.85 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 7 | 0.85 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 4 | 0.85 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 4 | 0.85 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 5 | 0.85 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 10 | 0.85 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 10 | 0.85 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 10 | 0.85 |
| (1,2567) | 1:B:105:ALA:HA | 1:B:108:GLU:HB2 | 5 | 0.85 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 5 | 0.85 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 3 | 0.85 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 3 | 0.85 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 5 | 0.85 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 10 | 0.85 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 4 | 0.85 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 4 | 0.85 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 6 | 0.85 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 6 | 0.84 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 6 | 0.84 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 5 | 0.84 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 9 | 0.84 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE1 | 6 | 0.84 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE2 | 6 | 0.84 |
| (1,728) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HA | 2 | 0.84 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 9 | 0.84 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 7 | 0.84 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 7 | 0.84 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 7 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3566) | 1:B:168:PRO:HD2 | 1:B:169:MET:HA | 10 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 2 | 0.84 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 2 | 0.84 |
| (1,3293) | 1:B:148:VAL:HG11 | 1:B:169:MET:HB2 | 5 | 0.84 |
| (1,3293) | 1:B:148:VAL:HG12 | 1:B:169:MET:HB2 | 5 | 0.84 |
| (1,3293) | 1:B:148:VAL:HG13 | 1:B:169:MET:HB2 | 5 | 0.84 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 1 | 0.84 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 9 | 0.84 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 3 | 0.84 |
| (1,2298) | 1:B:93:ASP:HA | 1:B:169:MET:HG2 | 8 | 0.84 |
| (1,2284) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB2 | 3 | 0.84 |
| (1,2284) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB2 | 3 | 0.84 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 9 | 0.84 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 9 | 0.84 |
| (1,7) | 1:A:90:HIS:HB2 | 1:A:91:THR:HA | 1 | 0.83 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 5 | 0.83 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 7 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 6 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 6 | 0.83 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 6 | 0.83 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 7 | 0.83 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 7 | 0.83 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 7 | 0.83 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 6 | 0.83 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 6 | 0.83 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 6 | 0.83 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 6 | 0.83 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 9 | 0.83 |
| (1,3003) | 1:B:126:GLU:HG2 | 1:B:135:SER:HA | 4 | 0.83 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 2 | 0.83 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 7 | 0.83 |
| (1,2290) | 1:B:90:HIS:HB3 | 1:B:91:THR:HA | 5 | 0.83 |
| (1,2012) | 1:A:172:LEU:H | 1:A:171:LYS:HA | 10 | 0.83 |
| (1,1998) | 1:A:169:MET:H | 1:A:169:MET:HB2 | 3 | 0.83 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 4 | 0.83 |
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 2 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 1 | 0.83 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 1 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 1 | 0.83 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 4 | 0.83 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 4 | 0.83 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 4 | 0.83 |
| (1,839) | 1:A:140:ARG:HB2 | 1:A:140:ARG:HD2 | 3 | 0.82 |
| (1,839) | 1:A:140:ARG:HB3 | 1:A:140:ARG:HD2 | 3 | 0.82 |
| (1,827) | 1:A:139:THR:HA | 1:A:140:ARG:HG2 | 3 | 0.82 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE1 | 2 | 0.82 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE2 | 2 | 0.82 |
| (1,728) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HA | 5 | 0.82 |
| (1,722) | 1:A:126:GLU:HG2 | 1:A:135:SER:HA | 5 | 0.82 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 3 | 0.82 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 3 | 0.82 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 3 | 0.82 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 1 | 0.82 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 1 | 0.82 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 1 | 0.82 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 6 | 0.82 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 8 | 0.82 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE2 | 7 | 0.82 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE3 | 7 | 0.82 |
| (1,3583) | 1:B:169:MET:HB3 | 1:B:171:LYS:HE3 | 7 | 0.82 |
| (1,3583) | 1:B:169:MET:HB2 | 1:B:171:LYS:HE2 | 7 | 0.82 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG11 | 10 | 0.82 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG12 | 10 | 0.82 |
| (1,3408) | 1:B:155:SER:HB3 | 1:B:165:VAL:HG13 | 10 | 0.82 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 8 | 0.82 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 8 | 0.82 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 8 | 0.82 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 8 | 0.82 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 2 | 0.82 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 6 | 0.82 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 6 | 0.82 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE1 | 7 | 0.82 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE2 | 7 | 0.82 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 2 | 0.82 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE2 | 3 | 0.82 |
| (1,2002) | 1:A:169:MET:H | 1:A:171:LYS:HE3 | 3 | 0.82 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 8 | 0.82 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 5 | 0.82 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 5 | 0.82 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 10 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 10 | 0.82 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 10 | 0.82 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 10 | 0.82 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 6 | 0.82 |
| (1,1) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HA | 7 | 0.82 |
| (1,1) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HA | 7 | 0.82 |
| (1,1) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HA | 7 | 0.82 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 2 | 0.81 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD3 | 6 | 0.81 |
| (1,949) | 1:A:145:PRO:HB2 | 1:A:146:PRO:HD2 | 6 | 0.81 |
| (1,4280) | 1:B:169:MET:H | 1:B:169:MET:HB3 | 7 | 0.81 |
| (1,4272) | 1:B:169:MET:H | 1:B:95:TRP:HA | 6 | 0.81 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 5 | 0.81 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 5 | 0.81 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 5 | 0.81 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 5 | 0.81 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 5 | 0.81 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 5 | 0.81 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 1 | 0.81 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 1 | 0.81 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 1 | 0.81 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 5 | 0.81 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 7 | 0.81 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 7 | 0.81 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 7 | 0.81 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 10 | 0.81 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 10 | 0.81 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 10 | 0.81 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 4 | 0.81 |
| (1,2991) | 1:B:126:GLU:HA | 1:B:135:SER:HB2 | 4 | 0.81 |
| (1,2969) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB3 | 9 | 0.81 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE1 | 1 | 0.81 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE2 | 1 | 0.81 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 8 | 0.81 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 8 | 0.81 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 8 | 0.81 |
| (1,1998) | 1:A:169:MET:H | 1:A:169:MET:HB2 | 4 | 0.81 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 5 | 0.81 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 5 | 0.81 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 4 | 0.81 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 10 | 0.81 |
| (1,1482) | 1:A:114:LYS:H | 1:A:115:ASP:HB2 | 5 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 5 | 0.81 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 1 | 0.8 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 1 | 0.8 |
| (1,688) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB3 | 3 | 0.8 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG21 | 10 | 0.8 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG22 | 10 | 0.8 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG23 | 10 | 0.8 |
| (1,4197) | 1:B:162:THR:H | 1:B:102:ASN:HB3 | 10 | 0.8 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 5 | 0.8 |
| (1,3763) | 1:B:114:LYS:H | 1:B:115:ASP:HB2 | 6 | 0.8 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 3 | 0.8 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD2 | 9 | 0.8 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD3 | 9 | 0.8 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 4 | 0.8 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 4 | 0.8 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 4 | 0.8 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 10 | 0.8 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 10 | 0.8 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 10 | 0.8 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 8 | 0.8 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 8 | 0.8 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 8 | 0.8 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 9 | 0.8 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 9 | 0.8 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 9 | 0.8 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 9 | 0.8 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 9 | 0.8 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 9 | 0.8 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 10 | 0.8 |
| (1,2281) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 10 | 0.8 |
| (1,2148) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 10 | 0.8 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD11 | 10 | 0.8 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD12 | 10 | 0.8 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD13 | 10 | 0.8 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD21 | 10 | 0.8 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD22 | 10 | 0.8 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD23 | 10 | 0.8 |
| (1,2) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HB3 | 1 | 0.8 |
| (1,2) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HB3 | 1 | 0.8 |
| (1,2) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HB3 | 1 | 0.8 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 1 | 0.8 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 1 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 1 | 0.8 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 9 | 0.79 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 3 | 0.79 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 9 | 0.79 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 9 | 0.79 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 9 | 0.79 |
| (1,3346) | 1:B:152:GLN:HB2 | 1:B:169:MET:HA | 4 | 0.79 |
| (1,3345) | 1:B:152:GLN:HB2 | 1:B:168:PRO:HD3 | 3 | 0.79 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 7 | 0.79 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 7 | 0.79 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 4 | 0.79 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 10 | 0.79 |
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 8 | 0.79 |
| (1,2969) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB3 | 6 | 0.79 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 6 | 0.79 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 6 | 0.79 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 6 | 0.79 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 2 | 0.79 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 2 | 0.79 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 2 | 0.79 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 1 | 0.79 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 6 | 0.79 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 6 | 0.79 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 8 | 0.79 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 2 | 0.79 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 7 | 0.79 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 7 | 0.79 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 7 | 0.79 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 7 | 0.79 |
| (1,1) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HA | 6 | 0.79 |
| (1,1) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HA | 6 | 0.79 |
| (1,1) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HA | 6 | 0.79 |
| (1,827) | 1:A:139:THR:HA | 1:A:140:ARG:HG2 | 4 | 0.78 |
| (1,684) | 1:A:123:LYS:HA | 1:A:135:SER:HB3 | 2 | 0.78 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD11 | 7 | 0.78 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD12 | 7 | 0.78 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD13 | 7 | 0.78 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD21 | 7 | 0.78 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD22 | 7 | 0.78 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD23 | 7 | 0.78 |
| (1,4065) | 1:B:152:GLN:H | 1:B:149:ASP:HB3 | 5 | 0.78 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 8 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 10 | 0.78 |
| (1,3895) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB2 | 10 | 0.78 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 2 | 0.78 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 2 | 0.78 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 2 | 0.78 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 2 | 0.78 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 10 | 0.78 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 3 | 0.78 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 10 | 0.78 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 2 | 0.78 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 2 | 0.78 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 2 | 0.78 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 2 | 0.78 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 2 | 0.78 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 2 | 0.78 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 3 | 0.78 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG2 | 6 | 0.78 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG3 | 6 | 0.78 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 9 | 0.78 |
| (1,1799) | 1:A:152:GLN:HE21 | 1:A:152:GLN:HB3 | 6 | 0.78 |
| (1,1691) | 1:A:140:ARG:H | 1:A:120:ILE:HB | 9 | 0.78 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 10 | 0.78 |
| (1,990) | 1:A:148:VAL:HA | 1:A:169:MET:HB2 | 5 | 0.77 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 4 | 0.77 |
| (1,839) | 1:A:140:ARG:HB2 | 1:A:140:ARG:HD2 | 4 | 0.77 |
| (1,839) | 1:A:140:ARG:HB3 | 1:A:140:ARG:HD2 | 4 | 0.77 |
| (1,710) | 1:A:126:GLU:HA | 1:A:135:SER:HB2 | 7 | 0.77 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 10 | 0.77 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 4 | 0.77 |
| (1,4255) | 1:B:167:ALA:H | 1:B:95:TRP:HB3 | 4 | 0.77 |
| (1,4080) | 1:B:152:GLN:HE21 | 1:B:152:GLN:HB3 | 3 | 0.77 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 1 | 0.77 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 4 | 0.77 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 4 | 0.77 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 1 | 0.77 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 1 | 0.77 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 1 | 0.77 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 1 | 0.77 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 1 | 0.77 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 1 | 0.77 |
| (1,3346) | 1:B:152:GLN:HB2 | 1:B:169:MET:HA | 9 | 0.77 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 8 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 8 | 0.77 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 1 | 0.77 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 1 | 0.77 |
| (1,2969) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB3 | 5 | 0.77 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 7 | 0.77 |
| (1,2322) | 1:B:94:ARG:HB3 | 1:B:167:ALA:HA | 10 | 0.77 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 4 | 0.77 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 6 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 7 | 0.77 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 7 | 0.77 |
| (1,99) | 1:A:96:ARG:HB3 | 1:A:164:THR:HB | 7 | 0.76 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 5 | 0.76 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 3 | 0.76 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 4 | 0.76 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE1 | 8 | 0.76 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE2 | 8 | 0.76 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 5 | 0.76 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 4 | 0.76 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 4 | 0.76 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 4 | 0.76 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 3 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 3 | 0.76 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 3 | 0.76 |
| (1,4272) | 1:B:169:MET:H | 1:B:95:TRP:HA | 5 | 0.76 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 10 | 0.76 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 7 | 0.76 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 10 | 0.76 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 10 | 0.76 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 10 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 9 | 0.76 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 9 | 0.76 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 10 | 0.76 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 10 | 0.76 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 10 | 0.76 |
| (1,3271) | 1:B:148:VAL:HA | 1:B:169:MET:HB2 | 4 | 0.76 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 1 | 0.76 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 1 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 1 | 0.76 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 7 | 0.76 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 7 | 0.76 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 7 | 0.76 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 7 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 5 | 0.76 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 1 | 0.76 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 1 | 0.76 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 5 | 0.76 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 3 | 0.76 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG3 | 7 | 0.76 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG2 | 7 | 0.76 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 6 | 0.75 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 6 | 0.75 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 6 | 0.75 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 3 | 0.75 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 3 | 0.75 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 3 | 0.75 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 3 | 0.75 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 3 | 0.75 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 3 | 0.75 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD2 | 7 | 0.75 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD3 | 7 | 0.75 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 5 | 0.75 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 5 | 0.75 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 5 | 0.75 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 5 | 0.75 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 5 | 0.75 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 5 | 0.75 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 1 | 0.75 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 1 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 1 | 0.75 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 1 | 0.75 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 7 | 0.75 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 7 | 0.75 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 7 | 0.75 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 4 | 0.75 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 4 | 0.75 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 4 | 0.75 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 4 | 0.75 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 4 | 0.75 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 4 | 0.75 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 10 | 0.75 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 10 | 0.75 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 10 | 0.75 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 3 | 0.75 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 3 | 0.75 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 3 | 0.75 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 6 | 0.75 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 6 | 0.75 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 6 | 0.75 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 5 | 0.75 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 5 | 0.75 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 5 | 0.75 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 5 | 0.75 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 5 | 0.75 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 5 | 0.75 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 10 | 0.74 |
| (1,8) | 1:A:90:HIS:HB2 | 1:A:91:THR:HG21 | 4 | 0.74 |
| (1,8) | 1:A:90:HIS:HB2 | 1:A:91:THR:HG22 | 4 | 0.74 |
| (1,8) | 1:A:90:HIS:HB2 | 1:A:91:THR:HG23 | 4 | 0.74 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 1 | 0.74 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 1 | 0.74 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 1 | 0.74 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB1 | 3 | 0.74 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB2 | 3 | 0.74 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB3 | 3 | 0.74 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 9 | 0.74 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 9 | 0.74 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 9 | 0.74 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 9 | 0.74 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 9 | 0.74 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 9 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 4 | 0.74 |
| (1,385) | 1:A:109:LEU:HD21 | 1:A:161:GLY:HA3 | 4 | 0.74 |
| (1,385) | 1:A:109:LEU:HD22 | 1:A:161:GLY:HA3 | 4 | 0.74 |
| (1,385) | 1:A:109:LEU:HD23 | 1:A:161:GLY:HA3 | 4 | 0.74 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 9 | 0.74 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 3 | 0.74 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 3 | 0.74 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 3 | 0.74 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 9 | 0.74 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 3 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 4 | 0.74 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 4 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 1 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 1 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 1 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 1 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 1 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 1 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 8 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 8 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 8 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 8 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 8 | 0.74 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 8 | 0.74 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 9 | 0.74 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 9 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 3 | 0.74 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 2 | 0.74 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 7 | 0.74 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 7 | 0.74 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 7 | 0.74 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 7 | 0.74 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 7 | 0.74 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 7 | 0.74 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 3 | 0.74 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 3 | 0.74 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 3 | 0.74 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 4 | 0.73 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 5 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 5 | 0.73 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 5 | 0.73 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 8 | 0.73 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 8 | 0.73 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 8 | 0.73 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 8 | 0.73 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 8 | 0.73 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 8 | 0.73 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 1 | 0.73 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 2 | 0.73 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 10 | 0.73 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 10 | 0.73 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 10 | 0.73 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 10 | 0.73 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 4 | 0.73 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 3 | 0.73 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 3 | 0.73 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 3 | 0.73 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 3 | 0.73 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 3 | 0.73 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 3 | 0.73 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 4 | 0.73 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 10 | 0.73 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 7 | 0.73 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 6 | 0.73 |
| (1,1608) | 1:A:128:GLN:HE22 | 1:A:128:GLN:HB2 | 7 | 0.73 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 4 | 0.73 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 4 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 4 | 0.73 |
| (1,1) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HA | 9 | 0.73 |
| (1,1) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HA | 9 | 0.73 |
| (1,1) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HA | 9 | 0.73 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 8 | 0.72 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE1 | 2 | 0.72 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE2 | 2 | 0.72 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 6 | 0.72 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD11 | 8 | 0.72 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD12 | 8 | 0.72 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD13 | 8 | 0.72 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD21 | 8 | 0.72 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD22 | 8 | 0.72 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD23 | 8 | 0.72 |
| (1,4048) | 1:B:149:ASP:H | 1:B:170:PRO:HG3 | 5 | 0.72 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD1 | 3 | 0.72 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD2 | 3 | 0.72 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 1 | 0.72 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 9 | 0.72 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 9 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 8 | 0.72 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 8 | 0.72 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 9 | 0.72 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 5 | 0.72 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 5 | 0.72 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 5 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 3 | 0.72 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 3 | 0.72 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 3 | 0.72 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 6 | 0.72 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 6 | 0.72 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 5 | 0.72 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 5 | 0.72 |
| (1,3003) | 1:B:126:GLU:HG2 | 1:B:135:SER:HA | 8 | 0.72 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG21 | 3 | 0.72 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG22 | 3 | 0.72 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG23 | 3 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 3 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 3 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 3 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 3 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 3 | 0.72 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 3 | 0.72 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD2 | 2 | 0.72 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD3 | 2 | 0.72 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 1 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 1 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 1 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 1 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 2 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 2 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 2 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 10 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 10 | 0.72 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 10 | 0.72 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 10 | 0.71 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE1 | 9 | 0.71 |
| (1,763) | 1:A:128:GLN:HG3 | 1:A:133:TYR:HE2 | 9 | 0.71 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 1 | 0.71 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 1 | 0.71 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 1 | 0.71 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 2 | 0.71 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 2 | 0.71 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 10 | 0.71 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 6 | 0.71 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 6 | 0.71 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 6 | 0.71 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 6 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 10 | 0.71 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 8 | 0.71 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 8 | 0.71 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 8 | 0.71 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 9 | 0.71 |
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 7 | 0.71 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 9 | 0.71 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE1 | 10 | 0.71 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE2 | 10 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 8 | 0.71 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 8 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 5 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 5 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 5 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 5 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 5 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 5 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 10 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 10 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 10 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 10 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 10 | 0.71 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 10 | 0.71 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 1 | 0.71 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 1 | 0.71 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 1 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 4 | 0.71 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 4 | 0.71 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 4 | 0.71 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 4 | 0.71 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 4 | 0.71 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 4 | 0.71 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 7 | 0.71 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 7 | 0.71 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 7 | 0.71 |
| (1,2213) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 1 | 0.71 |
| (1,2213) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 5 | 0.71 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2081) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 1 | 0.71 |
| (1,2081) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 5 | 0.71 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 2 | 0.71 |
| (1,2000) | 1:A:169:MET:H | 1:A:169:MET:HG3 | 7 | 0.71 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 8 | 0.71 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 8 | 0.71 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 8 | 0.71 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 4 | 0.71 |
| (1,1318) | 1:A:171:LYS:HA | 1:A:171:LYS:HD2 | 2 | 0.71 |
| (1,1318) | 1:A:171:LYS:HA | 1:A:171:LYS:HD3 | 2 | 0.71 |
| (1,1012) | 1:A:148:VAL:HG11 | 1:A:169:MET:HB2 | 5 | 0.71 |
| (1,1012) | 1:A:148:VAL:HG12 | 1:A:169:MET:HB2 | 5 | 0.71 |
| (1,1012) | 1:A:148:VAL:HG13 | 1:A:169:MET:HB2 | 5 | 0.71 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 5 | 0.7 |
| (1,9) | 1:A:90:HIS:HB3 | 1:A:91:THR:HA | 10 | 0.7 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 4 | 0.7 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 1 | 0.7 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB1 | 1 | 0.7 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB2 | 1 | 0.7 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB3 | 1 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB1 | 9 | 0.7 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB2 | 9 | 0.7 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB3 | 9 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 6 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 6 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 6 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 6 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 6 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 6 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 10 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 10 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 10 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 10 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 10 | 0.7 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 10 | 0.7 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 8 | 0.7 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 2 | 0.7 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 2 | 0.7 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 5 | 0.7 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 5 | 0.7 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 1 | 0.7 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 1 | 0.7 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 2 | 0.7 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 2 | 0.7 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 3 | 0.7 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 3 | 0.7 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 6 | 0.7 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 9 | 0.7 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 7 | 0.7 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 7 | 0.7 |
| (1,2988) | 1:B:126:GLU:HA | 1:B:133:TYR:HB3 | 6 | 0.7 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 1 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 7 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 7 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 9 | 0.7 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 9 | 0.7 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 1 | 0.7 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 1 | 0.7 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 4 | 0.7 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 10 | 0.7 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 10 | 0.7 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 10 | 0.7 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 3 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 3 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD21 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD22 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD23 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD21 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD22 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD23 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD21 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD22 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD23 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD11 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD12 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HD13 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD11 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD12 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HD13 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD11 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD12 | 5 | 0.7 |
| (1,1175) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HD13 | 5 | 0.7 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 7 | 0.69 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 6 | 0.69 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 5 | 0.69 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 7 | 0.69 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 9 | 0.69 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 9 | 0.69 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD22 | 8 | 0.69 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD21 | 8 | 0.69 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD2 | 3 | 0.69 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD3 | 3 | 0.69 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 1 | 0.69 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 1 | 0.69 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 1 | 0.69 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 2 | 0.69 |
| (1,3096) | 1:B:136:ARG:HG3 | 1:B:138:PHE:HA | 10 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 1 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 5 | 0.69 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 5 | 0.69 |
| (1,2545) | 1:B:100:ASP:HB2 | 1:B:162:THR:HB | 1 | 0.69 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 4 | 0.69 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 6 | 0.69 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 5 | 0.69 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 7 | 0.69 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 3 | 0.69 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 3 | 0.69 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 3 | 0.69 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 3 | 0.69 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 3 | 0.69 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 3 | 0.69 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 1 | 0.69 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 9 | 0.69 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 9 | 0.68 |
| (1,684) | 1:A:123:LYS:HA | 1:A:135:SER:HB3 | 3 | 0.68 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 8 | 0.68 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD2 | 5 | 0.68 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD3 | 5 | 0.68 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 9 | 0.68 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 7 | 0.68 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE1 | 1 | 0.68 |
| (1,3044) | 1:B:128:GLN:HG3 | 1:B:133:TYR:HE2 | 1 | 0.68 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 5 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 5 | 0.68 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 5 | 0.68 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG21 | 9 | 0.68 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG22 | 9 | 0.68 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG23 | 9 | 0.68 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG21 | 10 | 0.68 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG22 | 10 | 0.68 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG23 | 10 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 1 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 2 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 2 | 0.68 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 2 | 0.68 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 5 | 0.68 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 5 | 0.68 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 5 | 0.68 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 6 | 0.68 |
| (1,232) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HG12 | 7 | 0.68 |
| (1,232) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HG12 | 7 | 0.68 |
| (1,232) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HG12 | 7 | 0.68 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD2 | 8 | 0.68 |
| (1,2007) | 1:A:171:LYS:H | 1:A:170:PRO:HD3 | 8 | 0.68 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 2 | 0.68 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 2 | 0.68 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 2 | 0.68 |
| (1,1691) | 1:A:140:ARG:H | 1:A:120:ILE:HB | 6 | 0.68 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 2 | 0.68 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 8 | 0.68 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 9 | 0.68 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 2 | 0.68 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 2 | 0.68 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 2 | 0.68 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 2 | 0.68 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 2 | 0.68 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 2 | 0.68 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 9 | 0.68 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 9 | 0.68 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 9 | 0.68 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 4 | 0.68 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 9 | 0.67 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 9 | 0.67 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 9 | 0.67 |
| (1,710) | 1:A:126:GLU:HA | 1:A:135:SER:HB2 | 9 | 0.67 |
| (1,688) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB3 | 5 | 0.67 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB1 | 7 | 0.67 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB2 | 7 | 0.67 |
| (1,63) | 1:A:95:TRP:HB2 | 1:A:167:ALA:HB3 | 7 | 0.67 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 6 | 0.67 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 6 | 0.67 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 6 | 0.67 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 5 | 0.67 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 7 | 0.67 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 4 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 8 | 0.67 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 8 | 0.67 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 8 | 0.67 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 8 | 0.67 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 8 | 0.67 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 8 | 0.67 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 8 | 0.67 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 8 | 0.67 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 8 | 0.67 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 5 | 0.67 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 5 | 0.67 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 9 | 0.67 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 4 | 0.67 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 7 | 0.67 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 7 | 0.67 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 7 | 0.67 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 7 | 0.67 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 7 | 0.67 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 7 | 0.67 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD3 | 3 | 0.67 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD2 | 3 | 0.67 |
| (1,2561) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA3 | 1 | 0.67 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 5 | 0.67 |
| (1,2322) | 1:B:94:ARG:HB3 | 1:B:167:ALA:HA | 1 | 0.67 |
| (1,232) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HG12 | 6 | 0.67 |
| (1,232) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HG12 | 6 | 0.67 |
| (1,232) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HG12 | 6 | 0.67 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 9 | 0.67 |
| (1,1614) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB2 | 3 | 0.67 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 1 | 0.67 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 5 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 1 | 0.67 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 9 | 0.66 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 9 | 0.66 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 2 | 0.66 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 3 | 0.66 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 9 | 0.66 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 6 | 0.66 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 6 | 0.66 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 6 | 0.66 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 7 | 0.66 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 8 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 6 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 6 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 6 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 6 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 6 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 6 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 9 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 9 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 9 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 9 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 9 | 0.66 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 9 | 0.66 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 7 | 0.66 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 7 | 0.66 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 7 | 0.66 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 7 | 0.66 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 7 | 0.66 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 9 | 0.66 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 9 | 0.66 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 5 | 0.66 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 5 | 0.66 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 5 | 0.66 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 3 | 0.66 |
| (1,3009) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HA | 4 | 0.66 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 6 | 0.66 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 7 | 0.66 |
| (1,2325) | 1:B:94:ARG:HG2 | 1:B:166:GLU:HB2 | 4 | 0.66 |
| (1,2325) | 1:B:94:ARG:HG3 | 1:B:166:GLU:HB2 | 4 | 0.66 |
| (1,2314) | 1:B:94:ARG:HA | 1:B:169:MET:HB2 | 2 | 0.66 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 6 | 0.66 |
| (1,2157) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 10 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2025) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 10 | 0.66 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 7 | 0.66 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB2 | 10 | 0.66 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB3 | 10 | 0.66 |
| (1,1920) | 1:A:162:THR:H | 1:A:158:SER:HB2 | 4 | 0.66 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 4 | 0.66 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 4 | 0.66 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 4 | 0.66 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 5 | 0.66 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 1 | 0.66 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 6 | 0.66 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG21 | 4 | 0.66 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG22 | 4 | 0.66 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG23 | 4 | 0.66 |
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 9 | 0.66 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 7 | 0.66 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 7 | 0.66 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 7 | 0.66 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 2 | 0.66 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 10 | 0.66 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 4 | 0.65 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 4 | 0.65 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 7 | 0.65 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 7 | 0.65 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 1 | 0.65 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 4 | 0.65 |
| (1,710) | 1:A:126:GLU:HA | 1:A:135:SER:HB2 | 3 | 0.65 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 2 | 0.65 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 2 | 0.65 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 2 | 0.65 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 6 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 6 | 0.65 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 10 | 0.65 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 10 | 0.65 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 10 | 0.65 |
| (1,4285) | 1:B:171:LYS:H | 1:B:169:MET:HA | 9 | 0.65 |
| (1,4267) | 1:B:167:ALA:H | 1:B:169:MET:H | 8 | 0.65 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD1 | 4 | 0.65 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD2 | 4 | 0.65 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 6 | 0.65 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 6 | 0.65 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 6 | 0.65 |
| (1,3346) | 1:B:152:GLN:HB2 | 1:B:169:MET:HA | 10 | 0.65 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 5 | 0.65 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 5 | 0.65 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 3 | 0.65 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG3 | 6 | 0.65 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG2 | 6 | 0.65 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 4 | 0.65 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 5 | 0.65 |
| (1,2004) | 1:A:171:LYS:H | 1:A:169:MET:HA | 5 | 0.65 |
| (1,1691) | 1:A:140:ARG:H | 1:A:120:ILE:HB | 2 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 6 | 0.65 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 6 | 0.65 |
| (1,1277) | 1:A:168:PRO:HA | 1:A:169:MET:HG3 | 4 | 0.65 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 5 | 0.65 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 5 | 0.65 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 5 | 0.65 |
| (1,1085) | 1:A:153:VAL:HG11 | 1:A:155:SER:HB3 | 1 | 0.65 |
| (1,1085) | 1:A:153:VAL:HG12 | 1:A:155:SER:HB3 | 1 | 0.65 |
| (1,1085) | 1:A:153:VAL:HG13 | 1:A:155:SER:HB3 | 1 | 0.65 |
| (1,1085) | 1:A:153:VAL:HG21 | 1:A:155:SER:HB3 | 1 | 0.65 |
| (1,1085) | 1:A:153:VAL:HG22 | 1:A:155:SER:HB3 | 1 | 0.65 |
| (1,1085) | 1:A:153:VAL:HG23 | 1:A:155:SER:HB3 | 1 | 0.65 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 8 | 0.64 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 3 | 0.64 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 8 | 0.64 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 1 | 0.64 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 1 | 0.64 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 5 | 0.64 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 5 | 0.64 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 8 | 0.64 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 8 | 0.64 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 5 | 0.64 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 7 | 0.64 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 8 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 8 | 0.64 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 8 | 0.64 |
| (1,4286) | 1:B:171:LYS:H | 1:B:170:PRO:HB2 | 4 | 0.64 |
| (1,4286) | 1:B:171:LYS:H | 1:B:170:PRO:HB3 | 4 | 0.64 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 8 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 3 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 3 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 3 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 3 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 3 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 3 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 4 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 4 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 4 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 4 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 4 | 0.64 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 4 | 0.64 |
| (1,3763) | 1:B:114:LYS:H | 1:B:115:ASP:HB2 | 4 | 0.64 |
| (1,3569) | 1:B:169:MET:HA | 1:B:169:MET:HG2 | 6 | 0.64 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 2 | 0.64 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 4 | 0.64 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 4 | 0.64 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 4 | 0.64 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 1 | 0.64 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 1 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 10 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 10 | 0.64 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 10 | 0.64 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 2 | 0.64 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG21 | 2 | 0.64 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG22 | 2 | 0.64 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG23 | 2 | 0.64 |
| (1,2282) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HA | 9 | 0.64 |
| (1,2282) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HA | 9 | 0.64 |
| (1,2282) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HA | 9 | 0.64 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG2 | 6 | 0.64 |
| (1,1899) | 1:A:160:GLU:H | 1:A:160:GLU:HG3 | 6 | 0.64 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 8 | 0.64 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 4 | 0.64 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 4 | 0.64 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 4 | 0.64 |
| (1,1322) | 1:A:94:ARG:H | 1:A:93:ASP:HB2 | 6 | 0.64 |
| (1,1288) | 1:A:169:MET:HA | 1:A:169:MET:HG2 | 9 | 0.64 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 1 | 0.64 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 7 | 0.63 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 2 | 0.63 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 2 | 0.63 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 2 | 0.63 |
| (1,7) | 1:A:90:HIS:HB2 | 1:A:91:THR:HA | 2 | 0.63 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD2 | 9 | 0.63 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD3 | 9 | 0.63 |
| (1,4255) | 1:B:167:ALA:H | 1:B:95:TRP:HB3 | 7 | 0.63 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 10 | 0.63 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 10 | 0.63 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 10 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 2 | 0.63 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 2 | 0.63 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 2 | 0.63 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 2 | 0.63 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 2 | 0.63 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 2 | 0.63 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 7 | 0.63 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 7 | 0.63 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 7 | 0.63 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 7 | 0.63 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 7 | 0.63 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 7 | 0.63 |
| (1,3603) | 1:B:94:ARG:H | 1:B:93:ASP:HB2 | 1 | 0.63 |
| (1,3566) | 1:B:168:PRO:HD2 | 1:B:169:MET:HA | 9 | 0.63 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 10 | 0.63 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 10 | 0.63 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 6 | 0.63 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 6 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG13 | 8 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG13 | 8 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG13 | 8 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG13 | 8 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG13 | 8 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG13 | 8 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG13 | 10 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG13 | 10 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG13 | 10 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG13 | 10 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG13 | 10 | 0.63 |
| (1,2716) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG13 | 10 | 0.63 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 2 | 0.63 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 2 | 0.63 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 2 | 0.63 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 4 | 0.63 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 10 | 0.63 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 3 | 0.63 |
| (1,2314) | 1:B:94:ARG:HA | 1:B:169:MET:HB2 | 6 | 0.63 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB1 | 4 | 0.63 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB2 | 4 | 0.63 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB3 | 4 | 0.63 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 3 | 0.63 |
| (1,2284) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB2 | 6 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2284) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB2 | 6 | 0.63 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 6 | 0.63 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 7 | 0.63 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG21 | 6 | 0.63 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG22 | 6 | 0.63 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG23 | 6 | 0.63 |
| (1,1318) | 1:A:171:LYS:HA | 1:A:171:LYS:HD2 | 10 | 0.63 |
| (1,1318) | 1:A:171:LYS:HA | 1:A:171:LYS:HD3 | 10 | 0.63 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 5 | 0.63 |
| (1,839) | 1:A:140:ARG:HB2 | 1:A:140:ARG:HD2 | 9 | 0.62 |
| (1,839) | 1:A:140:ARG:HB3 | 1:A:140:ARG:HD2 | 9 | 0.62 |
| (1,743) | 1:A:127:ARG:HB3 | 1:A:127:ARG:HD2 | 5 | 0.62 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 6 | 0.62 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE1 | 10 | 0.62 |
| (1,642) | 1:A:120:ILE:HG13 | 1:A:142:TYR:HE2 | 10 | 0.62 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 1 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 1 | 0.62 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 1 | 0.62 |
| (1,4048) | 1:B:149:ASP:H | 1:B:170:PRO:HG3 | 4 | 0.62 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 7 | 0.62 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 9 | 0.62 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 5 | 0.62 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 5 | 0.62 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 5 | 0.62 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 5 | 0.62 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 5 | 0.62 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 5 | 0.62 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 7 | 0.62 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 7 | 0.62 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 7 | 0.62 |
| (1,3569) | 1:B:169:MET:HA | 1:B:169:MET:HG2 | 3 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 3 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 3 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 3 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 3 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 3 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 3 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 10 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 10 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 10 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 10 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 10 | 0.62 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 10 | 0.62 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 10 | 0.62 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 10 | 0.62 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 10 | 0.62 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 9 | 0.62 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 1 | 0.62 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 1 | 0.62 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 1 | 0.62 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 7 | 0.62 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 7 | 0.62 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 7 | 0.62 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 5 | 0.62 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 5 | 0.62 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 1 | 0.62 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 1 | 0.62 |
| (1,31) | 1:A:94:ARG:HA | 1:A:168:PRO:HD2 | 2 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2716) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG13 | 1 | 0.62 |
| (1,2716) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG13 | 1 | 0.62 |
| (1,2716) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG13 | 1 | 0.62 |
| (1,2716) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG13 | 1 | 0.62 |
| (1,2716) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG13 | 1 | 0.62 |
| (1,2716) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG13 | 1 | 0.62 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 3 | 0.62 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 3 | 0.62 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 3 | 0.62 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 6 | 0.62 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 6 | 0.62 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 6 | 0.62 |
| (1,2513) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HG12 | 6 | 0.62 |
| (1,2513) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HG12 | 6 | 0.62 |
| (1,2513) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HG12 | 6 | 0.62 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 9 | 0.62 |
| (1,2290) | 1:B:90:HIS:HB3 | 1:B:91:THR:HA | 8 | 0.62 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 8 | 0.62 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 1 | 0.62 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 1 | 0.62 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 1 | 0.62 |
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 3 | 0.62 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 7 | 0.62 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 7 | 0.62 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 7 | 0.62 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 7 | 0.62 |
| (1,1114) | 1:A:155:SER:HB2 | 1:A:163:LEU:HA | 2 | 0.62 |
| (1,968) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA3 | 3 | 0.61 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 5 | 0.61 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 3 | 0.61 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 3 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 7 | 0.61 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 8 | 0.61 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 10 | 0.61 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 6 | 0.61 |
| (1,4080) | 1:B:152:GLN:HE21 | 1:B:152:GLN:HB3 | 10 | 0.61 |
| (1,4024) | 1:B:148:VAL:H | 1:B:146:PRO:HB3 | 5 | 0.61 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 2 | 0.61 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 2 | 0.61 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 2 | 0.61 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 10 | 0.61 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 6 | 0.61 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 8 | 0.61 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 8 | 0.61 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 8 | 0.61 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 7 | 0.61 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG2 | 3 | 0.61 |
| (1,3243) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HG3 | 3 | 0.61 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 4 | 0.61 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 4 | 0.61 |
| (1,3118) | 1:B:140:ARG:HA | 1:B:140:ARG:HD3 | 3 | 0.61 |
| (1,3116) | 1:B:139:THR:HG21 | 1:B:141:LYS:HE2 | 7 | 0.61 |
| (1,3116) | 1:B:139:THR:HG22 | 1:B:141:LYS:HE2 | 7 | 0.61 |
| (1,3116) | 1:B:139:THR:HG23 | 1:B:141:LYS:HE2 | 7 | 0.61 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 2 | 0.61 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 5 | 0.61 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 5 | 0.61 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 5 | 0.61 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG21 | 5 | 0.61 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG22 | 5 | 0.61 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG23 | 5 | 0.61 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG21 | 8 | 0.61 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG22 | 8 | 0.61 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG23 | 8 | 0.61 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 4 | 0.61 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 4 | 0.61 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 4 | 0.61 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 7 | 0.61 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 5 | 0.61 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 1 | 0.61 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 10 | 0.61 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 10 | 0.61 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 10 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 10 | 0.61 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 10 | 0.61 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 10 | 0.61 |
| (1,1413) | 1:A:108:GLU:H | 1:A:106:PRO:HB3 | 7 | 0.61 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD22 | 4 | 0.61 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD21 | 4 | 0.61 |
| (1,1288) | 1:A:169:MET:HA | 1:A:169:MET:HG2 | 1 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 1 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 1 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 1 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 1 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 1 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 1 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 6 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 6 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 6 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 6 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 6 | 0.61 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 6 | 0.61 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 8 | 0.61 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 8 | 0.61 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 8 | 0.61 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 3 | 0.61 |
| (1,723) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB2 | 4 | 0.6 |
| (1,723) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB2 | 8 | 0.6 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 3 | 0.6 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 10 | 0.6 |
| (1,3972) | 1:B:140:ARG:H | 1:B:120:ILE:HB | 2 | 0.6 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 4 | 0.6 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 2 | 0.6 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 2 | 0.6 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 2 | 0.6 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 4 | 0.6 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 4 | 0.6 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 4 | 0.6 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 3 | 0.6 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 3 | 0.6 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 8 | 0.6 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 8 | 0.6 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 8 | 0.6 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE1 | 9 | 0.6 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE2 | 9 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 3 | 0.6 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 3 | 0.6 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 3 | 0.6 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 2 | 0.6 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 3 | 0.6 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 3 | 0.6 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 5 | 0.6 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB2 | 5 | 0.6 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB3 | 5 | 0.6 |
| (1,1916) | 1:A:162:THR:H | 1:A:102:ASN:HB3 | 4 | 0.6 |
| (1,1656) | 1:A:134:ILE:H | 1:A:127:ARG:HG3 | 1 | 0.6 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 1 | 0.6 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 10 | 0.6 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 10 | 0.6 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 10 | 0.6 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 10 | 0.6 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 10 | 0.6 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 10 | 0.6 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 10 | 0.6 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 10 | 0.6 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 10 | 0.6 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 4 | 0.6 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 2 | 0.59 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG2 | 10 | 0.59 |
| (1,962) | 1:A:145:PRO:HD2 | 1:A:146:PRO:HG3 | 10 | 0.59 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 3 | 0.59 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 3 | 0.59 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 3 | 0.59 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 2 | 0.59 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 9 | 0.59 |
| (1,626) | 1:A:120:ILE:HA | 1:A:120:ILE:HG13 | 3 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,435) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG13 | 3 | 0.59 |
| (1,435) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG13 | 3 | 0.59 |
| (1,435) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG13 | 3 | 0.59 |
| (1,435) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG13 | 3 | 0.59 |
| (1,435) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG13 | 3 | 0.59 |
| (1,435) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG13 | 3 | 0.59 |
| (1,4267) | 1:B:167:ALA:H | 1:B:169:MET:H | 7 | 0.59 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 10 | 0.59 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 7 | 0.59 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 7 | 0.59 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 7 | 0.59 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 1 | 0.59 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 1 | 0.59 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 1 | 0.59 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 4 | 0.59 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 5 | 0.59 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 5 | 0.59 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 8 | 0.59 |
| (1,2907) | 1:B:120:ILE:HA | 1:B:120:ILE:HG13 | 4 | 0.59 |
| (1,2716) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG13 | 7 | 0.59 |
| (1,2716) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG13 | 7 | 0.59 |
| (1,2716) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG13 | 7 | 0.59 |
| (1,2716) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG13 | 7 | 0.59 |
| (1,2716) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG13 | 7 | 0.59 |
| (1,2716) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG13 | 7 | 0.59 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 2 | 0.59 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 2 | 0.59 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 2 | 0.59 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 9 | 0.59 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 9 | 0.59 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 9 | 0.59 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 8 | 0.59 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 8 | 0.59 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 8 | 0.59 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 8 | 0.59 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 8 | 0.59 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 8 | 0.59 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 1 | 0.59 |
| (1,2346) | 1:B:95:TRP:HB3 | 1:B:95:TRP:HE3 | 1 | 0.59 |
| (1,232) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HG12 | 9 | 0.59 |
| (1,232) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HG12 | 9 | 0.59 |
| (1,232) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HG12 | 9 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 10 | 0.59 |
| (1,2151) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2151) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2151) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2151) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2151) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2151) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 10 | 0.59 |
| (1,2019) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2019) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2019) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2019) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2019) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2019) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB2 | 8 | 0.59 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 3 | 0.59 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 3 | 0.59 |
| (1,1277) | 1:A:168:PRO:HA | 1:A:169:MET:HG3 | 3 | 0.59 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB1 | 9 | 0.59 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB2 | 9 | 0.59 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB3 | 9 | 0.59 |
| (1,841) | 1:A:140:ARG:HG2 | 1:A:142:TYR:HE1 | 8 | 0.58 |
| (1,841) | 1:A:140:ARG:HG2 | 1:A:142:TYR:HE2 | 8 | 0.58 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 8 | 0.58 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 1 | 0.58 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 1 | 0.58 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 1 | 0.58 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 1 | 0.58 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 2 | 0.58 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 2 | 0.58 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 2 | 0.58 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 6 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD21 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD22 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD23 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD21 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD22 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD23 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD21 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD22 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD23 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD11 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD12 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HD13 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD11 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD12 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HD13 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD11 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD12 | 1 | 0.58 |
| (1,3456) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HD13 | 1 | 0.58 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 4 | 0.58 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 10 | 0.58 |
| (1,3249) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA3 | 9 | 0.58 |
| (1,3248) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA2 | 6 | 0.58 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 3 | 0.58 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 6 | 0.58 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 2 | 0.58 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 3 | 0.58 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 7 | 0.58 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 7 | 0.58 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 7 | 0.58 |
| (1,2930) | 1:B:120:ILE:HG21 | 1:B:140:ARG:HA | 6 | 0.58 |
| (1,2930) | 1:B:120:ILE:HG22 | 1:B:140:ARG:HA | 6 | 0.58 |
| (1,2930) | 1:B:120:ILE:HG23 | 1:B:140:ARG:HA | 6 | 0.58 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG21 | 6 | 0.58 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG22 | 6 | 0.58 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG23 | 6 | 0.58 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG11 | 6 | 0.58 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG12 | 6 | 0.58 |
| (1,2670) | 1:B:110:THR:HA | 1:B:111:VAL:HG13 | 6 | 0.58 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 8 | 0.58 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 8 | 0.58 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 8 | 0.58 |
| (1,2561) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA3 | 9 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2283) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HB3 | 8 | 0.58 |
| (1,2283) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HB3 | 8 | 0.58 |
| (1,2283) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HB3 | 8 | 0.58 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 8 | 0.58 |
| (1,16) | 1:A:93:ASP:HA | 1:A:94:ARG:HD2 | 1 | 0.58 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 7 | 0.58 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG3 | 3 | 0.58 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG2 | 3 | 0.58 |
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 1 | 0.58 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 4 | 0.58 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 4 | 0.58 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 4 | 0.58 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 4 | 0.58 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 4 | 0.58 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 4 | 0.58 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 4 | 0.57 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 2 | 0.57 |
| (1,733) | 1:A:126:GLU:HG3 | 1:A:135:SER:HB3 | 3 | 0.57 |
| (1,65) | 1:A:95:TRP:HB3 | 1:A:95:TRP:HE3 | 7 | 0.57 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 1 | 0.57 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 1 | 0.57 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 1 | 0.57 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 1 | 0.57 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 1 | 0.57 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 1 | 0.57 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 4 | 0.57 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 1 | 0.57 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 1 | 0.57 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 1 | 0.57 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 2 | 0.57 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 2 | 0.57 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 2 | 0.57 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 1 | 0.57 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 1 | 0.57 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 6 | 0.57 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 6 | 0.57 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 6 | 0.57 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 5 | 0.57 |
| (1,3005) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB3 | 8 | 0.57 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 3 | 0.57 |
| (1,2969) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB3 | 2 | 0.57 |
| (1,2907) | 1:B:120:ILE:HA | 1:B:120:ILE:HG13 | 8 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 8 | 0.57 |
| (1,2346) | 1:B:95:TRP:HB3 | 1:B:95:TRP:HE3 | 7 | 0.57 |
| (1,2193) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 10 | 0.57 |
| (1,2061) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 10 | 0.57 |
| (1,1691) | 1:A:140:ARG:H | 1:A:120:ILE:HB | 7 | 0.57 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 7 | 0.57 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 5 | 0.57 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 9 | 0.57 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 9 | 0.57 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 9 | 0.57 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 5 | 0.57 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB1 | 7 | 0.57 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB2 | 7 | 0.57 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB3 | 7 | 0.57 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 6 | 0.57 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 6 | 0.57 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 2 | 0.56 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 10 | 0.56 |
| (1,839) | 1:A:140:ARG:HB2 | 1:A:140:ARG:HD2 | 5 | 0.56 |
| (1,839) | 1:A:140:ARG:HB3 | 1:A:140:ARG:HD2 | 5 | 0.56 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 2 | 0.56 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 2 | 0.56 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 2 | 0.56 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 9 | 0.56 |
| (1,65) | 1:A:95:TRP:HB3 | 1:A:95:TRP:HE3 | 4 | 0.56 |
| (1,626) | 1:A:120:ILE:HA | 1:A:120:ILE:HG13 | 1 | 0.56 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 8 | 0.56 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 9 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 9 | 0.56 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 9 | 0.56 |
| (1,4080) | 1:B:152:GLN:HE21 | 1:B:152:GLN:HB3 | 9 | 0.56 |
| (1,4024) | 1:B:148:VAL:H | 1:B:146:PRO:HB3 | 6 | 0.56 |
| (1,3972) | 1:B:140:ARG:H | 1:B:120:ILE:HB | 3 | 0.56 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD1 | 2 | 0.56 |
| (1,3911) | 1:B:129:ASP:H | 1:B:133:TYR:HD2 | 2 | 0.56 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG21 | 7 | 0.56 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG22 | 7 | 0.56 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG23 | 7 | 0.56 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG11 | 7 | 0.56 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG12 | 7 | 0.56 |
| (1,389) | 1:A:110:THR:HA | 1:A:111:VAL:HG13 | 7 | 0.56 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 1 | 0.56 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 7 | 0.56 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 6 | 0.56 |
| (1,33) | 1:A:94:ARG:HA | 1:A:169:MET:HB2 | 2 | 0.56 |
| (1,3293) | 1:B:148:VAL:HG11 | 1:B:169:MET:HB2 | 4 | 0.56 |
| (1,3293) | 1:B:148:VAL:HG12 | 1:B:169:MET:HB2 | 4 | 0.56 |
| (1,3293) | 1:B:148:VAL:HG13 | 1:B:169:MET:HB2 | 4 | 0.56 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 7 | 0.56 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 7 | 0.56 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 5 | 0.56 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 5 | 0.56 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 3 | 0.56 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 9 | 0.56 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 7 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 6 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 6 | 0.56 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 6 | 0.56 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 5 | 0.56 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 5 | 0.56 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 5 | 0.56 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 8 | 0.56 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 3 | 0.56 |
| (1,2325) | 1:B:94:ARG:HG2 | 1:B:166:GLU:HB2 | 5 | 0.56 |
| (1,2325) | 1:B:94:ARG:HG3 | 1:B:166:GLU:HB2 | 5 | 0.56 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 10 | 0.56 |
| (1,2169) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 9 | 0.56 |
| (1,2037) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 9 | 0.56 |
| (1,1916) | 1:A:162:THR:H | 1:A:102:ASN:HB3 | 2 | 0.56 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 2 | 0.56 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 4 | 0.56 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 2 | 0.56 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 2 | 0.56 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 10 | 0.56 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 10 | 0.56 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD22 | 2 | 0.56 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD21 | 2 | 0.56 |
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 7 | 0.56 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 8 | 0.56 |
| (1,1114) | 1:A:155:SER:HB2 | 1:A:163:LEU:HA | 1 | 0.56 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 3 | 0.56 |
| (1,104) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HA | 3 | 0.56 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 1 | 0.55 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 7 | 0.55 |
| (1,770) | 1:A:129:ASP:HB3 | 1:A:130:GLU:HA | 8 | 0.55 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB1 | 8 | 0.55 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB2 | 8 | 0.55 |
| (1,77) | 1:A:95:TRP:HE3 | 1:A:167:ALA:HB3 | 8 | 0.55 |
| (1,723) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB2 | 1 | 0.55 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 1 | 0.55 |
| (1,626) | 1:A:120:ILE:HA | 1:A:120:ILE:HG13 | 8 | 0.55 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 6 | 0.55 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 5 | 0.55 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 5 | 0.55 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 5 | 0.55 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 5 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 5 | 0.55 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 5 | 0.55 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 5 | 0.55 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 8 | 0.55 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 8 | 0.55 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 8 | 0.55 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 5 | 0.55 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 10 | 0.55 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 5 | 0.55 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 5 | 0.55 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 5 | 0.55 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 5 | 0.55 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 5 | 0.55 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 5 | 0.55 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 3 | 0.55 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 3 | 0.55 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 3 | 0.55 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 2 | 0.55 |
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 2 | 0.55 |
| (1,2907) | 1:B:120:ILE:HA | 1:B:120:ILE:HG13 | 7 | 0.55 |
| (1,2322) | 1:B:94:ARG:HB3 | 1:B:167:ALA:HA | 3 | 0.55 |
| (1,2313) | 1:B:94:ARG:HA | 1:B:168:PRO:HD3 | 2 | 0.55 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 7 | 0.55 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 2 | 0.55 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 9 | 0.55 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 4 | 0.55 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 10 | 0.55 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 6 | 0.55 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 6 | 0.55 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 6 | 0.55 |
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD22 | 7 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1367) | 1:A:102:ASN:H | 1:A:102:ASN:HD21 | 7 | 0.55 |
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 3 | 0.55 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 9 | 0.55 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 9 | 0.55 |
| (1,699) | 1:A:125:GLU:HA | 1:A:125:GLU:HG2 | 10 | 0.54 |
| (1,65) | 1:A:95:TRP:HB3 | 1:A:95:TRP:HE3 | 10 | 0.54 |
| (1,626) | 1:A:120:ILE:HA | 1:A:120:ILE:HG13 | 5 | 0.54 |
| (1,626) | 1:A:120:ILE:HA | 1:A:120:ILE:HG13 | 10 | 0.54 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD11 | 1 | 0.54 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD12 | 1 | 0.54 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD13 | 1 | 0.54 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD21 | 1 | 0.54 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD22 | 1 | 0.54 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD23 | 1 | 0.54 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE2 | 3 | 0.54 |
| (1,4283) | 1:B:169:MET:H | 1:B:171:LYS:HE3 | 3 | 0.54 |
| (1,4280) | 1:B:169:MET:H | 1:B:169:MET:HB3 | 2 | 0.54 |
| (1,4084) | 1:B:152:GLN:HE21 | 1:B:168:PRO:HD2 | 3 | 0.54 |
| (1,4036) | 1:B:148:VAL:H | 1:B:170:PRO:HB2 | 9 | 0.54 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 8 | 0.54 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 9 | 0.54 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 9 | 0.54 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 9 | 0.54 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 9 | 0.54 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 9 | 0.54 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 9 | 0.54 |
| (1,3603) | 1:B:94:ARG:H | 1:B:93:ASP:HB2 | 8 | 0.54 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 7 | 0.54 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 7 | 0.54 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 7 | 0.54 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 7 | 0.54 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 7 | 0.54 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 7 | 0.54 |
| (1,3137) | 1:B:141:LYS:HG2 | 1:B:142:TYR:HB3 | 10 | 0.54 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 9 | 0.54 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 9 | 0.54 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 10 | 0.54 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 1 | 0.54 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD11 | 1 | 0.54 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD12 | 1 | 0.54 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD13 | 1 | 0.54 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 8 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 8 | 0.54 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 8 | 0.54 |
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 9 | 0.54 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 9 | 0.54 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 9 | 0.54 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 3 | 0.54 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 3 | 0.54 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 3 | 0.54 |
| (1,2299) | 1:B:93:ASP:HB2 | 1:B:94:ARG:HA | 3 | 0.54 |
| (1,2193) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 5 | 0.54 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2061) | 1:B:134:ILE:HA | 1:A:140:ARG:HD2 | 5 | 0.54 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 10 | 0.54 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 9 | 0.54 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB2 | 5 | 0.54 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB3 | 5 | 0.54 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 7 | 0.54 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 9 | 0.54 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 9 | 0.54 |
| (1,1766) | 1:A:149:ASP:H | 1:A:169:MET:HG3 | 7 | 0.54 |
| (1,1756) | 1:A:148:VAL:H | 1:A:170:PRO:HG3 | 7 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 5 | 0.54 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 8 | 0.54 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 8 | 0.54 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 8 | 0.54 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 8 | 0.54 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 8 | 0.54 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 8 | 0.54 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 7 | 0.54 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 10 | 0.54 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 10 | 0.54 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 10 | 0.53 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 4 | 0.53 |
| (1,699) | 1:A:125:GLU:HA | 1:A:125:GLU:HG2 | 3 | 0.53 |
| (1,688) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB3 | 8 | 0.53 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 10 | 0.53 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 9 | 0.53 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 6 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 4 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 4 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 4 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 4 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 4 | 0.53 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 4 | 0.53 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 4 | 0.53 |
| (1,3491) | 1:B:160:GLU:HB2 | 1:B:162:THR:HB | 10 | 0.53 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 7 | 0.53 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 7 | 0.53 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 7 | 0.53 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 5 | 0.53 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 1 | 0.53 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 4 | 0.53 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 6 | 0.53 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 6 | 0.53 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 6 | 0.53 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 5 | 0.53 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 5 | 0.53 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 5 | 0.53 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 9 | 0.53 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 10 | 0.53 |
| (1,2980) | 1:B:125:GLU:HA | 1:B:125:GLU:HG2 | 7 | 0.53 |
| (1,2907) | 1:B:120:ILE:HA | 1:B:120:ILE:HG13 | 1 | 0.53 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 6 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 6 | 0.53 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 6 | 0.53 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 10 | 0.53 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 10 | 0.53 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 10 | 0.53 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 2 | 0.53 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 10 | 0.53 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 5 | 0.53 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 5 | 0.53 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 5 | 0.53 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 7 | 0.53 |
| (1,2285) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB3 | 10 | 0.53 |
| (1,2285) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB3 | 10 | 0.53 |
| (1,2000) | 1:A:169:MET:H | 1:A:169:MET:HG3 | 2 | 0.53 |
| (1,1691) | 1:A:140:ARG:H | 1:A:120:ILE:HB | 4 | 0.53 |
| (1,1514) | 1:A:118:VAL:H | 1:A:119:GLU:HG3 | 1 | 0.53 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 10 | 0.52 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 7 | 0.52 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 6 | 0.52 |
| (1,4287) | 1:B:171:LYS:H | 1:B:170:PRO:HG2 | 5 | 0.52 |
| (1,4287) | 1:B:171:LYS:H | 1:B:170:PRO:HG3 | 5 | 0.52 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 2 | 0.52 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 2 | 0.52 |
| (1,4093) | 1:B:152:GLN:HE22 | 1:B:168:PRO:HD3 | 2 | 0.52 |
| (1,3895) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB2 | 3 | 0.52 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 5 | 0.52 |
| (1,3612) | 1:B:95:TRP:H | 1:B:95:TRP:HB2 | 9 | 0.52 |
| (1,3491) | 1:B:160:GLU:HB2 | 1:B:162:THR:HB | 8 | 0.52 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 8 | 0.52 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 2 | 0.52 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 2 | 0.52 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 2 | 0.52 |
| (1,2974) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB3 | 6 | 0.52 |
| (1,2971) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HB2 | 10 | 0.52 |
| (1,2907) | 1:B:120:ILE:HA | 1:B:120:ILE:HG13 | 9 | 0.52 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 4 | 0.52 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 1 | 0.52 |
| (1,2790) | 1:B:114:LYS:HA | 1:B:114:LYS:HB2 | 5 | 0.52 |
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 2 | 0.52 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 2 | 0.52 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 2 | 0.52 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 2 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 2 | 0.52 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 4 | 0.52 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD11 | 1 | 0.52 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD12 | 1 | 0.52 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD13 | 1 | 0.52 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 6 | 0.52 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 9 | 0.52 |
| (1,2346) | 1:B:95:TRP:HB3 | 1:B:95:TRP:HE3 | 8 | 0.52 |
| (1,2200) | 1:B:134:ILE:HG21 | 1:A:140:ARG:HD3 | 3 | 0.52 |
| (1,2200) | 1:B:134:ILE:HG22 | 1:A:140:ARG:HD3 | 3 | 0.52 |
| (1,2200) | 1:B:134:ILE:HG23 | 1:A:140:ARG:HD3 | 3 | 0.52 |
| (1,2068) | 1:B:134:ILE:HG21 | 1:A:140:ARG:HD3 | 3 | 0.52 |
| (1,2068) | 1:B:134:ILE:HG22 | 1:A:140:ARG:HD3 | 3 | 0.52 |
| (1,2068) | 1:B:134:ILE:HG23 | 1:A:140:ARG:HD3 | 3 | 0.52 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 10 | 0.52 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD11 | 1 | 0.52 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD12 | 1 | 0.52 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD13 | 1 | 0.52 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD21 | 1 | 0.52 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD22 | 1 | 0.52 |
| (1,2014) | 1:A:172:LEU:H | 1:A:172:LEU:HD23 | 1 | 0.52 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 6 | 0.52 |
| (1,1642) | 1:A:132:GLY:H | 1:A:129:ASP:HB2 | 2 | 0.52 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 3 | 0.52 |
| (1,1210) | 1:A:160:GLU:HB2 | 1:A:162:THR:HB | 4 | 0.52 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 8 | 0.51 |
| (1,722) | 1:A:126:GLU:HG2 | 1:A:135:SER:HA | 6 | 0.51 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 8 | 0.51 |
| (1,699) | 1:A:125:GLU:HA | 1:A:125:GLU:HG2 | 1 | 0.51 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 6 | 0.51 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 4 | 0.51 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG11 | 1 | 0.51 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG12 | 1 | 0.51 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG13 | 1 | 0.51 |
| (1,4262) | 1:B:167:ALA:H | 1:B:166:GLU:HB2 | 6 | 0.51 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 7 | 0.51 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 4 | 0.51 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 7 | 0.51 |
| (1,3889) | 1:B:128:GLN:HE22 | 1:B:128:GLN:HB2 | 10 | 0.51 |
| (1,3848) | 1:B:123:LYS:H | 1:B:109:LEU:HG | 6 | 0.51 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 6 | 0.51 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 6 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 6 | 0.51 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 7 | 0.51 |
| (1,3613) | 1:B:95:TRP:H | 1:B:95:TRP:HE3 | 7 | 0.51 |
| (1,3604) | 1:B:94:ARG:H | 1:B:93:ASP:HB3 | 7 | 0.51 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 4 | 0.51 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 4 | 0.51 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 1 | 0.51 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 1 | 0.51 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 1 | 0.51 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 10 | 0.51 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 10 | 0.51 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 10 | 0.51 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE1 | 3 | 0.51 |
| (1,2923) | 1:B:120:ILE:HG13 | 1:B:142:TYR:HE2 | 3 | 0.51 |
| (1,2907) | 1:B:120:ILE:HA | 1:B:120:ILE:HG13 | 10 | 0.51 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 3 | 0.51 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 7 | 0.51 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 8 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG13 | 4 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG13 | 4 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG13 | 4 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG13 | 4 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG13 | 4 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG13 | 4 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG13 | 9 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG13 | 9 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG13 | 9 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG13 | 9 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG13 | 9 | 0.51 |
| (1,2716) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG13 | 9 | 0.51 |
| (1,2561) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA3 | 3 | 0.51 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 1 | 0.51 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 8 | 0.51 |
| (1,2282) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HA | 10 | 0.51 |
| (1,2282) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HA | 10 | 0.51 |
| (1,2282) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HA | 10 | 0.51 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 8 | 0.51 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 8 | 0.51 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 6 | 0.51 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 4 | 0.51 |
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 6 | 0.51 |
| (1,18) | 1:A:93:ASP:HB2 | 1:A:94:ARG:HA | 6 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1799) | 1:A:152:GLN:HE21 | 1:A:152:GLN:HB3 | 7 | 0.51 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 10 | 0.51 |
| (1,1193) | 1:A:158:SER:HB3 | 1:A:160:GLU:HB3 | 2 | 0.51 |
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 10 | 0.51 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 7 | 0.51 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD21 | 9 | 0.51 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD22 | 9 | 0.51 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD23 | 9 | 0.51 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD11 | 9 | 0.51 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD12 | 9 | 0.51 |
| (1,1156) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HD13 | 9 | 0.51 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 3 | 0.5 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 6 | 0.5 |
| (1,699) | 1:A:125:GLU:HA | 1:A:125:GLU:HG2 | 7 | 0.5 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 4 | 0.5 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 4 | 0.5 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 4 | 0.5 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 2 | 0.5 |
| (1,44) | 1:A:94:ARG:HG2 | 1:A:166:GLU:HB2 | 2 | 0.5 |
| (1,44) | 1:A:94:ARG:HG3 | 1:A:166:GLU:HB2 | 2 | 0.5 |
| (1,4269) | 1:B:169:MET:H | 1:B:94:ARG:HA | 7 | 0.5 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 10 | 0.5 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB1 | 7 | 0.5 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB2 | 7 | 0.5 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB3 | 7 | 0.5 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 10 | 0.5 |
| (1,4024) | 1:B:148:VAL:H | 1:B:146:PRO:HB3 | 8 | 0.5 |
| (1,3763) | 1:B:114:LYS:H | 1:B:115:ASP:HB2 | 7 | 0.5 |
| (1,3704) | 1:B:108:GLU:H | 1:B:123:LYS:HG2 | 2 | 0.5 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 1 | 0.5 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 3 | 0.5 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 8 | 0.5 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 7 | 0.5 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 6 | 0.5 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 10 | 0.5 |
| (1,3274) | 1:B:148:VAL:HA | 1:B:170:PRO:HG2 | 3 | 0.5 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG11 | 3 | 0.5 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG12 | 3 | 0.5 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG13 | 3 | 0.5 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG11 | 3 | 0.5 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG12 | 3 | 0.5 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG13 | 3 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD3 | 3 | 0.5 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD2 | 3 | 0.5 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 6 | 0.5 |
| (1,2980) | 1:B:125:GLU:HA | 1:B:125:GLU:HG2 | 5 | 0.5 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 2 | 0.5 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 5 | 0.5 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 9 | 0.5 |
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 6 | 0.5 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 6 | 0.5 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 6 | 0.5 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 7 | 0.5 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 1 | 0.5 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 1 | 0.5 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 1 | 0.5 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 4 | 0.5 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 4 | 0.5 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 4 | 0.5 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 8 | 0.5 |
| (1,2473) | 1:B:98:SER:HB3 | 1:B:99:LEU:HD21 | 3 | 0.5 |
| (1,2473) | 1:B:98:SER:HB3 | 1:B:99:LEU:HD22 | 3 | 0.5 |
| (1,2473) | 1:B:98:SER:HB3 | 1:B:99:LEU:HD23 | 3 | 0.5 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 4 | 0.5 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 4 | 0.5 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 4 | 0.5 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 1 | 0.5 |
| (1,2281) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 3 | 0.5 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2148) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 3 | 0.5 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 9 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 9 | 0.5 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 4 | 0.5 |
| (1,2000) | 1:A:169:MET:H | 1:A:169:MET:HG3 | 9 | 0.5 |
| (1,18) | 1:A:93:ASP:HB2 | 1:A:94:ARG:HA | 4 | 0.5 |
| (1,1654) | 1:A:134:ILE:H | 1:A:127:ARG:HB2 | 3 | 0.5 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 2 | 0.5 |
| (1,1331) | 1:A:95:TRP:H | 1:A:95:TRP:HB2 | 8 | 0.5 |
| (1,1322) | 1:A:94:ARG:H | 1:A:93:ASP:HB2 | 4 | 0.5 |
| (1,1193) | 1:A:158:SER:HB3 | 1:A:160:GLU:HB3 | 4 | 0.5 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 8 | 0.5 |
| (1,710) | 1:A:126:GLU:HA | 1:A:135:SER:HB2 | 5 | 0.49 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 3 | 0.49 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 3 | 0.49 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 3 | 0.49 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 8 | 0.49 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 2 | 0.49 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 3 | 0.49 |
| (1,3460) | 1:B:157:LEU:HD21 | 1:B:163:LEU:HB3 | 7 | 0.49 |
| (1,3460) | 1:B:157:LEU:HD22 | 1:B:163:LEU:HB3 | 7 | 0.49 |
| (1,3460) | 1:B:157:LEU:HD23 | 1:B:163:LEU:HB3 | 7 | 0.49 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 4 | 0.49 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 4 | 0.49 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 4 | 0.49 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 4 | 0.49 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 4 | 0.49 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 4 | 0.49 |
| (1,3436) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HA | 1 | 0.49 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 2 | 0.49 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 2 | 0.49 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 2 | 0.49 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 2 | 0.49 |
| (1,3116) | 1:B:139:THR:HG21 | 1:B:141:LYS:HE2 | 5 | 0.49 |
| (1,3116) | 1:B:139:THR:HG22 | 1:B:141:LYS:HE2 | 5 | 0.49 |
| (1,3116) | 1:B:139:THR:HG23 | 1:B:141:LYS:HE2 | 5 | 0.49 |
| (1,3116) | 1:B:139:THR:HG21 | 1:B:141:LYS:HE2 | 6 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3116) | 1:B:139:THR:HG22 | 1:B:141:LYS:HE2 | 6 | 0.49 |
| (1,3116) | 1:B:139:THR:HG23 | 1:B:141:LYS:HE2 | 6 | 0.49 |
| (1,2980) | 1:B:125:GLU:HA | 1:B:125:GLU:HG2 | 8 | 0.49 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 4 | 0.49 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 4 | 0.49 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 4 | 0.49 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 1 | 0.49 |
| (1,2790) | 1:B:114:LYS:HA | 1:B:114:LYS:HB2 | 3 | 0.49 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 2 | 0.49 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 2 | 0.49 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 7 | 0.49 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 7 | 0.49 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 7 | 0.49 |
| (1,2194) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 5 | 0.49 |
| (1,2062) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 5 | 0.49 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 6 | 0.49 |
| (1,1743) | 1:A:148:VAL:H | 1:A:146:PRO:HB3 | 6 | 0.49 |
| (1,1582) | 1:A:125:GLU:H | 1:A:124:HIS:HB2 | 10 | 0.49 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB1 | 2 | 0.49 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB2 | 2 | 0.49 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB3 | 2 | 0.49 |
| (1,99) | 1:A:96:ARG:HB3 | 1:A:164:THR:HB | 1 | 0.48 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 7 | 0.48 |
| (1,770) | 1:A:129:ASP:HB3 | 1:A:130:GLU:HA | 9 | 0.48 |
| (1,718) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HB3 | 10 | 0.48 |
| (1,688) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB3 | 7 | 0.48 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 3 | 0.48 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 3 | 0.48 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 3 | 0.48 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 3 | 0.48 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD2 | 3 | 0.48 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD3 | 3 | 0.48 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD2 | 7 | 0.48 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD3 | 7 | 0.48 |
| (1,4267) | 1:B:167:ALA:H | 1:B:169:MET:H | 4 | 0.48 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 4 | 0.48 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 8 | 0.48 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 8 | 0.48 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 5 | 0.48 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 5 | 0.48 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 5 | 0.48 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 1 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 1 | 0.48 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 1 | 0.48 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 1 | 0.48 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 1 | 0.48 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 1 | 0.48 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD21 | 5 | 0.48 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD22 | 5 | 0.48 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD23 | 5 | 0.48 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 1 | 0.48 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 3 | 0.48 |
| (1,3274) | 1:B:148:VAL:HA | 1:B:170:PRO:HG2 | 1 | 0.48 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 8 | 0.48 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 8 | 0.48 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 8 | 0.48 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 5 | 0.48 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 5 | 0.48 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 5 | 0.48 |
| (1,3137) | 1:B:141:LYS:HG2 | 1:B:142:TYR:HB3 | 8 | 0.48 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 3 | 0.48 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 3 | 0.48 |
| (1,2970) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HA | 10 | 0.48 |
| (1,2969) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB3 | 8 | 0.48 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 10 | 0.48 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 10 | 0.48 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 10 | 0.48 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 8 | 0.48 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 8 | 0.48 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 8 | 0.48 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 6 | 0.48 |
| (1,282) | 1:A:105:ALA:HA | 1:A:106:PRO:HB2 | 10 | 0.48 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 7 | 0.48 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 5 | 0.48 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 6 | 0.48 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 10 | 0.48 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 9 | 0.48 |
| (1,2325) | 1:B:94:ARG:HG2 | 1:B:166:GLU:HB2 | 7 | 0.48 |
| (1,2325) | 1:B:94:ARG:HG3 | 1:B:166:GLU:HB2 | 7 | 0.48 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 9 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 6 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 6 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 8 | 0.48 |
| (1,1640) | 1:A:132:GLY:H | 1:A:128:GLN:HG2 | 5 | 0.48 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 2 | 0.48 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 3 | 0.48 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 7 | 0.48 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 10 | 0.48 |
| (1,1) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HA | 1 | 0.48 |
| (1,1) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HA | 1 | 0.48 |
| (1,1) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HA | 1 | 0.48 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 6 | 0.47 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 6 | 0.47 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 6 | 0.47 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 8 | 0.47 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 8 | 0.47 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 8 | 0.47 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 1 | 0.47 |
| (1,690) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HB2 | 10 | 0.47 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 5 | 0.47 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 5 | 0.47 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 5 | 0.47 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 4 | 0.47 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 4 | 0.47 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 4 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4255) | 1:B:167:ALA:H | 1:B:95:TRP:HB3 | 2 | 0.47 |
| (1,3895) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB2 | 6 | 0.47 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 2 | 0.47 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 1 | 0.47 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 1 | 0.47 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 4 | 0.47 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 4 | 0.47 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 4 | 0.47 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 9 | 0.47 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 9 | 0.47 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 9 | 0.47 |
| (1,3612) | 1:B:95:TRP:H | 1:B:95:TRP:HB2 | 5 | 0.47 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 6 | 0.47 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 6 | 0.47 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 6 | 0.47 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 8 | 0.47 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 8 | 0.47 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 8 | 0.47 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 1 | 0.47 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 7 | 0.47 |
| (1,2969) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB3 | 7 | 0.47 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 6 | 0.47 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 6 | 0.47 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 6 | 0.47 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 5 | 0.47 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG21 | 1 | 0.47 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG22 | 1 | 0.47 |
| (1,2795) | 1:B:115:ASP:HB2 | 1:B:143:THR:HG23 | 1 | 0.47 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 5 | 0.47 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 1 | 0.47 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 3 | 0.47 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 6 | 0.47 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 1 | 0.47 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG2 | 3 | 0.47 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG3 | 3 | 0.47 |
| (1,2) | 1:A:88:ILE:HG21 | 1:A:90:HIS:HB3 | 8 | 0.47 |
| (1,2) | 1:A:88:ILE:HG22 | 1:A:90:HIS:HB3 | 8 | 0.47 |
| (1,2) | 1:A:88:ILE:HG23 | 1:A:90:HIS:HB3 | 8 | 0.47 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB1 | 5 | 0.47 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB2 | 5 | 0.47 |
| (1,1843) | 1:A:154:SER:H | 1:A:167:ALA:HB3 | 5 | 0.47 |
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 7 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1331) | 1:A:95:TRP:H | 1:A:95:TRP:HB2 | 5 | 0.47 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 6 | 0.47 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 5 | 0.47 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 6 | 0.46 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 6 | 0.46 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 6 | 0.46 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 3 | 0.46 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 3 | 0.46 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 3 | 0.46 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 6 | 0.46 |
| (1,612) | 1:A:119:GLU:HA | 1:A:141:LYS:HE3 | 1 | 0.46 |
| (1,528) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HB | 4 | 0.46 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD2 | 6 | 0.46 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD3 | 6 | 0.46 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG21 | 10 | 0.46 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG22 | 10 | 0.46 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG23 | 10 | 0.46 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 5 | 0.46 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 10 | 0.46 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 10 | 0.46 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 10 | 0.46 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 6 | 0.46 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 8 | 0.46 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 8 | 0.46 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 8 | 0.46 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 8 | 0.46 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 8 | 0.46 |
| (1,3694) | 1:B:108:GLU:H | 1:B:106:PRO:HB3 | 2 | 0.46 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 9 | 0.46 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 4 | 0.46 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 4 | 0.46 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 4 | 0.46 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 2 | 0.46 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 1 | 0.46 |
| (1,3303) | 1:B:148:VAL:HG21 | 1:B:170:PRO:HG2 | 1 | 0.46 |
| (1,3303) | 1:B:148:VAL:HG22 | 1:B:170:PRO:HG2 | 1 | 0.46 |
| (1,3303) | 1:B:148:VAL:HG23 | 1:B:170:PRO:HG2 | 1 | 0.46 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 6 | 0.46 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 6 | 0.46 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 6 | 0.46 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 6 | 0.46 |
| (1,3027) | 1:B:128:GLN:HA | 1:B:128:GLN:HG3 | 1 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 3 | 0.46 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 3 | 0.46 |
| (1,2930) | 1:B:120:ILE:HG21 | 1:B:140:ARG:HA | 5 | 0.46 |
| (1,2930) | 1:B:120:ILE:HG22 | 1:B:140:ARG:HA | 5 | 0.46 |
| (1,2930) | 1:B:120:ILE:HG23 | 1:B:140:ARG:HA | 5 | 0.46 |
| (1,2893) | 1:B:119:GLU:HA | 1:B:141:LYS:HE3 | 9 | 0.46 |
| (1,2790) | 1:B:114:LYS:HA | 1:B:114:LYS:HB2 | 8 | 0.46 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 1 | 0.46 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 3 | 0.46 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 3 | 0.46 |
| (1,2563) | 1:B:105:ALA:HA | 1:B:106:PRO:HB2 | 9 | 0.46 |
| (1,2472) | 1:B:98:SER:HB3 | 1:B:99:LEU:HA | 3 | 0.46 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 5 | 0.46 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 2 | 0.46 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 7 | 0.46 |
| (1,2194) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 10 | 0.46 |
| (1,2062) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 10 | 0.46 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD2 | 10 | 0.46 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD3 | 10 | 0.46 |
| (1,1916) | 1:A:162:THR:H | 1:A:102:ASN:HB3 | 7 | 0.46 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 5 | 0.46 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 9 | 0.46 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 3 | 0.46 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 3 | 0.46 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 3 | 0.46 |
| (1,1664) | 1:A:135:SER:H | 1:A:134:ILE:HG13 | 5 | 0.46 |
| (1,1612) | 1:A:128:GLN:HE22 | 1:A:129:ASP:H | 7 | 0.46 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 8 | 0.46 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 4 | 0.46 |
| (1,1322) | 1:A:94:ARG:H | 1:A:93:ASP:HB2 | 9 | 0.46 |
| (1,1210) | 1:A:160:GLU:HB2 | 1:A:162:THR:HB | 7 | 0.46 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 5 | 0.46 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG11 | 9 | 0.46 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG12 | 9 | 0.46 |
| (1,1127) | 1:A:155:SER:HB3 | 1:A:165:VAL:HG13 | 9 | 0.46 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 10 | 0.46 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 7 | 0.46 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 8 | 0.46 |
| (1,728) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HA | 7 | 0.45 |
| (1,723) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB2 | 5 | 0.45 |
| (1,690) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HB2 | 4 | 0.45 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 6 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 6 | 0.45 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 6 | 0.45 |
| (1,528) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HB | 1 | 0.45 |
| (1,4280) | 1:B:169:MET:H | 1:B:169:MET:HB3 | 10 | 0.45 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 8 | 0.45 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 7 | 0.45 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 3 | 0.45 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 3 | 0.45 |
| (1,3748) | 1:B:113:THR:H | 1:B:112:LYS:HB2 | 8 | 0.45 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 6 | 0.45 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 5 | 0.45 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 9 | 0.45 |
| (1,3613) | 1:B:95:TRP:H | 1:B:95:TRP:HE3 | 1 | 0.45 |
| (1,3612) | 1:B:95:TRP:H | 1:B:95:TRP:HB2 | 10 | 0.45 |
| (1,3601) | 1:B:94:ARG:H | 1:B:92:ALA:HA | 5 | 0.45 |
| (1,3570) | 1:B:169:MET:HA | 1:B:169:MET:HG3 | 7 | 0.45 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 2 | 0.45 |
| (1,3460) | 1:B:157:LEU:HD21 | 1:B:163:LEU:HB3 | 4 | 0.45 |
| (1,3460) | 1:B:157:LEU:HD22 | 1:B:163:LEU:HB3 | 4 | 0.45 |
| (1,3460) | 1:B:157:LEU:HD23 | 1:B:163:LEU:HB3 | 4 | 0.45 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 7 | 0.45 |
| (1,3420) | 1:B:156:SER:HB3 | 1:B:157:LEU:HB3 | 10 | 0.45 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 8 | 0.45 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG11 | 10 | 0.45 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG12 | 10 | 0.45 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG13 | 10 | 0.45 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG11 | 10 | 0.45 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG12 | 10 | 0.45 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG13 | 10 | 0.45 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 4 | 0.45 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 4 | 0.45 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 4 | 0.45 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 5 | 0.45 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 5 | 0.45 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 5 | 0.45 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD3 | 2 | 0.45 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD2 | 2 | 0.45 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 9 | 0.45 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 2 | 0.45 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 5 | 0.45 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 5 | 0.45 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 5 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 6 | 0.45 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 6 | 0.45 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 6 | 0.45 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 5 | 0.45 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 9 | 0.45 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG3 | 2 | 0.45 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG2 | 2 | 0.45 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 10 | 0.45 |
| (1,2318) | 1:B:94:ARG:HB2 | 1:B:96:ARG:HA | 1 | 0.45 |
| (1,2314) | 1:B:94:ARG:HA | 1:B:169:MET:HB2 | 1 | 0.45 |
| (1,2013) | 1:A:172:LEU:H | 1:A:172:LEU:HB2 | 10 | 0.45 |
| (1,2013) | 1:A:172:LEU:H | 1:A:172:LEU:HB3 | 10 | 0.45 |
| (1,1924) | 1:A:162:THR:H | 1:A:160:GLU:HB2 | 2 | 0.45 |
| (1,1767) | 1:A:149:ASP:H | 1:A:170:PRO:HG3 | 4 | 0.45 |
| (1,1664) | 1:A:135:SER:H | 1:A:134:ILE:HG13 | 2 | 0.45 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 6 | 0.45 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 7 | 0.45 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG3 | 9 | 0.45 |
| (1,1301) | 1:A:169:MET:HB3 | 1:A:171:LYS:HG2 | 9 | 0.45 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 10 | 0.45 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 2 | 0.45 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB1 | 6 | 0.45 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB2 | 6 | 0.45 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB3 | 6 | 0.45 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 7 | 0.45 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 7 | 0.45 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 9 | 0.45 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 9 | 0.45 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 9 | 0.45 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 9 | 0.44 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 9 | 0.44 |
| (1,724) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB3 | 5 | 0.44 |
| (1,722) | 1:A:126:GLU:HG2 | 1:A:135:SER:HA | 9 | 0.44 |
| (1,718) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HB3 | 8 | 0.44 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 6 | 0.44 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 6 | 0.44 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 6 | 0.44 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 7 | 0.44 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 7 | 0.44 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 7 | 0.44 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 9 | 0.44 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 9 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 9 | 0.44 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 3 | 0.44 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 6 | 0.44 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 6 | 0.44 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 7 | 0.44 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 7 | 0.44 |
| (1,4296) | 1:B:173:ALA:H | 1:B:172:LEU:HG | 5 | 0.44 |
| (1,4294) | 1:B:172:LEU:H | 1:B:172:LEU:HB2 | 3 | 0.44 |
| (1,4294) | 1:B:172:LEU:H | 1:B:172:LEU:HB3 | 3 | 0.44 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD2 | 9 | 0.44 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD3 | 9 | 0.44 |
| (1,4272) | 1:B:169:MET:H | 1:B:95:TRP:HA | 4 | 0.44 |
| (1,4205) | 1:B:162:THR:H | 1:B:160:GLU:HB2 | 1 | 0.44 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 7 | 0.44 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 3 | 0.44 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 3 | 0.44 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 3 | 0.44 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 3 | 0.44 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 2 | 0.44 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 2 | 0.44 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 2 | 0.44 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 2 | 0.44 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 2 | 0.44 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 2 | 0.44 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 3 | 0.44 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 8 | 0.44 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 2 | 0.44 |
| (1,3607) | 1:B:94:ARG:H | 1:B:168:PRO:HA | 9 | 0.44 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD2 | 6 | 0.44 |
| (1,3599) | 1:B:171:LYS:HA | 1:B:171:LYS:HD3 | 6 | 0.44 |
| (1,3460) | 1:B:157:LEU:HD21 | 1:B:163:LEU:HB3 | 5 | 0.44 |
| (1,3460) | 1:B:157:LEU:HD22 | 1:B:163:LEU:HB3 | 5 | 0.44 |
| (1,3460) | 1:B:157:LEU:HD23 | 1:B:163:LEU:HB3 | 5 | 0.44 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 9 | 0.44 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 5 | 0.44 |
| (1,3345) | 1:B:152:GLN:HB2 | 1:B:168:PRO:HD3 | 7 | 0.44 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 7 | 0.44 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 7 | 0.44 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 7 | 0.44 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 10 | 0.44 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 10 | 0.44 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 2 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 2 | 0.44 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 2 | 0.44 |
| (1,2790) | 1:B:114:LYS:HA | 1:B:114:LYS:HB2 | 9 | 0.44 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 9 | 0.44 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 9 | 0.44 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 9 | 0.44 |
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 1 | 0.44 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 1 | 0.44 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 1 | 0.44 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 6 | 0.44 |
| (1,2551) | 1:B:101:VAL:HG11 | 1:B:102:ASN:HA | 5 | 0.44 |
| (1,2551) | 1:B:101:VAL:HG12 | 1:B:102:ASN:HA | 5 | 0.44 |
| (1,2551) | 1:B:101:VAL:HG13 | 1:B:102:ASN:HA | 5 | 0.44 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 3 | 0.44 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 6 | 0.44 |
| (1,2152) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2152) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2152) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2152) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2152) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2152) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2020) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2020) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2020) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2020) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2020) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,2020) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 6 | 0.44 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 7 | 0.44 |
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 5 | 0.44 |
| (1,1640) | 1:A:132:GLY:H | 1:A:128:GLN:HG2 | 4 | 0.44 |
| (1,1482) | 1:A:114:LYS:H | 1:A:115:ASP:HB2 | 9 | 0.44 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 6 | 0.44 |
| (1,1332) | 1:A:95:TRP:H | 1:A:95:TRP:HE3 | 10 | 0.44 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 8 | 0.44 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 8 | 0.44 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 8 | 0.44 |
| (1,1097) | 1:A:154:SER:HB3 | 1:A:155:SER:HA | 7 | 0.44 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 3 | 0.44 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 3 | 0.44 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 3 | 0.44 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 1 | 0.43 |
| (1,7) | 1:A:90:HIS:HB2 | 1:A:91:THR:HA | 8 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 4 | 0.43 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 4 | 0.43 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 4 | 0.43 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 8 | 0.43 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 8 | 0.43 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 8 | 0.43 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 8 | 0.43 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 9 | 0.43 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 9 | 0.43 |
| (1,435) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG13 | 5 | 0.43 |
| (1,435) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG13 | 5 | 0.43 |
| (1,435) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG13 | 5 | 0.43 |
| (1,435) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG13 | 5 | 0.43 |
| (1,435) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG13 | 5 | 0.43 |
| (1,435) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG13 | 5 | 0.43 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG21 | 1 | 0.43 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG22 | 1 | 0.43 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG23 | 1 | 0.43 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 9 | 0.43 |
| (1,4197) | 1:B:162:THR:H | 1:B:102:ASN:HB3 | 2 | 0.43 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 6 | 0.43 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 7 | 0.43 |
| (1,4084) | 1:B:152:GLN:HE21 | 1:B:168:PRO:HD2 | 1 | 0.43 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 2 | 0.43 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 10 | 0.43 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 10 | 0.43 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 10 | 0.43 |
| (1,3972) | 1:B:140:ARG:H | 1:B:120:ILE:HB | 5 | 0.43 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD1 | 1 | 0.43 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD2 | 1 | 0.43 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 4 | 0.43 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 4 | 0.43 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 7 | 0.43 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 7 | 0.43 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 7 | 0.43 |
| (1,370) | 1:A:109:LEU:HD11 | 1:A:122:GLY:HA3 | 5 | 0.43 |
| (1,370) | 1:A:109:LEU:HD12 | 1:A:122:GLY:HA3 | 5 | 0.43 |
| (1,370) | 1:A:109:LEU:HD13 | 1:A:122:GLY:HA3 | 5 | 0.43 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 5 | 0.43 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 5 | 0.43 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 6 | 0.43 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 6 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 6 | 0.43 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 8 | 0.43 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD21 | 2 | 0.43 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD22 | 2 | 0.43 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD23 | 2 | 0.43 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD11 | 2 | 0.43 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD12 | 2 | 0.43 |
| (1,3437) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HD13 | 2 | 0.43 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 1 | 0.43 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 1 | 0.43 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 1 | 0.43 |
| (1,3304) | 1:B:149:ASP:HA | 1:B:149:ASP:HB3 | 1 | 0.43 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 1 | 0.43 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 1 | 0.43 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 1 | 0.43 |
| (1,3299) | 1:B:148:VAL:HG21 | 1:B:168:PRO:HD3 | 10 | 0.43 |
| (1,3299) | 1:B:148:VAL:HG22 | 1:B:168:PRO:HD3 | 10 | 0.43 |
| (1,3299) | 1:B:148:VAL:HG23 | 1:B:168:PRO:HD3 | 10 | 0.43 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 1 | 0.43 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 1 | 0.43 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 1 | 0.43 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 2 | 0.43 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 2 | 0.43 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 2 | 0.43 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 7 | 0.43 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 2 | 0.43 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 6 | 0.43 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 2 | 0.43 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD21 | 1 | 0.43 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD22 | 1 | 0.43 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD23 | 1 | 0.43 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 8 | 0.43 |
| (1,2545) | 1:B:100:ASP:HB2 | 1:B:162:THR:HB | 9 | 0.43 |
| (1,2513) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HG12 | 2 | 0.43 |
| (1,2513) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HG12 | 2 | 0.43 |
| (1,2513) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HG12 | 2 | 0.43 |
| (1,2513) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HG12 | 5 | 0.43 |
| (1,2513) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HG12 | 5 | 0.43 |
| (1,2513) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HG12 | 5 | 0.43 |
| (1,247) | 1:A:99:LEU:HD21 | 1:A:140:ARG:HG3 | 3 | 0.43 |
| (1,247) | 1:A:99:LEU:HD22 | 1:A:140:ARG:HG3 | 3 | 0.43 |
| (1,247) | 1:A:99:LEU:HD23 | 1:A:140:ARG:HG3 | 3 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2383) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HB3 | 6 | 0.43 |
| (1,2314) | 1:B:94:ARG:HA | 1:B:169:MET:HB2 | 10 | 0.43 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 3 | 0.43 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 8 | 0.43 |
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 8 | 0.43 |
| (1,1799) | 1:A:152:GLN:HE21 | 1:A:152:GLN:HB3 | 3 | 0.43 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 4 | 0.43 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 4 | 0.43 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 9 | 0.43 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 8 | 0.43 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 1 | 0.43 |
| (1,1288) | 1:A:169:MET:HA | 1:A:169:MET:HG2 | 6 | 0.43 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 9 | 0.43 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 9 | 0.43 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 9 | 0.43 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 6 | 0.43 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 5 | 0.43 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 2 | 0.42 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 4 | 0.42 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 4 | 0.42 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 4 | 0.42 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 6 | 0.42 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 6 | 0.42 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 6 | 0.42 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 7 | 0.42 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 7 | 0.42 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 7 | 0.42 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 3 | 0.42 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 3 | 0.42 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 3 | 0.42 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 1 | 0.42 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 10 | 0.42 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 3 | 0.42 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 5 | 0.42 |
| (1,722) | 1:A:126:GLU:HG2 | 1:A:135:SER:HA | 3 | 0.42 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 5 | 0.42 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 10 | 0.42 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 10 | 0.42 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 10 | 0.42 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG21 | 1 | 0.42 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG22 | 1 | 0.42 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG23 | 1 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,49) | 1:A:94:ARG:HD3 | 1:A:168:PRO:HA | 8 | 0.42 |
| (1,4197) | 1:B:162:THR:H | 1:B:102:ASN:HB3 | 8 | 0.42 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 6 | 0.42 |
| (1,41) | 1:A:94:ARG:HB3 | 1:A:167:ALA:HA | 4 | 0.42 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 3 | 0.42 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 3 | 0.42 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 3 | 0.42 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 2 | 0.42 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 2 | 0.42 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 2 | 0.42 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 4 | 0.42 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 4 | 0.42 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 4 | 0.42 |
| (1,3895) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB2 | 7 | 0.42 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 10 | 0.42 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 4 | 0.42 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 4 | 0.42 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 4 | 0.42 |
| (1,3491) | 1:B:160:GLU:HB2 | 1:B:162:THR:HB | 2 | 0.42 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD3 | 2 | 0.42 |
| (1,3230) | 1:B:145:PRO:HB2 | 1:B:146:PRO:HD2 | 2 | 0.42 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 4 | 0.42 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 4 | 0.42 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 4 | 0.42 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 9 | 0.42 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 9 | 0.42 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 9 | 0.42 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 7 | 0.42 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 4 | 0.42 |
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 1 | 0.42 |
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 10 | 0.42 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 3 | 0.42 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 3 | 0.42 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 3 | 0.42 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 3 | 0.42 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 8 | 0.42 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 6 | 0.42 |
| (1,2468) | 1:B:98:SER:HB2 | 1:B:164:THR:HB | 8 | 0.42 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 6 | 0.42 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 7 | 0.42 |
| (1,2157) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 5 | 0.42 |
| (1,2025) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 5 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2008) | 1:A:171:LYS:H | 1:A:171:LYS:HA | 9 | 0.42 |
| (1,1974) | 1:A:167:ALA:H | 1:A:95:TRP:HB3 | 10 | 0.42 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 10 | 0.42 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 5 | 0.42 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 5 | 0.42 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 5 | 0.42 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 4 | 0.42 |
| (1,1552) | 1:A:121:THR:H | 1:A:120:ILE:HG12 | 10 | 0.42 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 9 | 0.42 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 3 | 0.42 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 1 | 0.42 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 1 | 0.42 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 1 | 0.42 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 3 | 0.41 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 3 | 0.41 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 3 | 0.41 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 8 | 0.41 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 8 | 0.41 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 8 | 0.41 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 6 | 0.41 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 2 | 0.41 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 2 | 0.41 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 2 | 0.41 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 3 | 0.41 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 3 | 0.41 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 3 | 0.41 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 5 | 0.41 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 5 | 0.41 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 5 | 0.41 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 7 | 0.41 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 7 | 0.41 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 7 | 0.41 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 9 | 0.41 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 9 | 0.41 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 9 | 0.41 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 3 | 0.41 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 3 | 0.41 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 3 | 0.41 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 3 | 0.41 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 3 | 0.41 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 5 | 0.41 |
| (1,435) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG13 | 1 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,435) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG13 | 1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG13 | 1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG13 | 1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG13 | 1 | 0.41 |
| (1,435) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG13 | 1 | 0.41 |
| (1,4285) | 1:B:171:LYS:H | 1:B:169:MET:HA | 6 | 0.41 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE1 | 8 | 0.41 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE2 | 8 | 0.41 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 5 | 0.41 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 5 | 0.41 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 5 | 0.41 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 6 | 0.41 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 10 | 0.41 |
| (1,3603) | 1:B:94:ARG:H | 1:B:93:ASP:HB2 | 7 | 0.41 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 6 | 0.41 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 9 | 0.41 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 10 | 0.41 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 8 | 0.41 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 8 | 0.41 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 8 | 0.41 |
| (1,3255) | 1:B:147:GLY:HA2 | 1:B:148:VAL:HG11 | 9 | 0.41 |
| (1,3255) | 1:B:147:GLY:HA2 | 1:B:148:VAL:HG12 | 9 | 0.41 |
| (1,3255) | 1:B:147:GLY:HA2 | 1:B:148:VAL:HG13 | 9 | 0.41 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 8 | 0.41 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 8 | 0.41 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 8 | 0.41 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 9 | 0.41 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 9 | 0.41 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 9 | 0.41 |
| (1,3092) | 1:B:136:ARG:HA | 1:B:136:ARG:HG2 | 10 | 0.41 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 9 | 0.41 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 10 | 0.41 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 10 | 0.41 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 2 | 0.41 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 2 | 0.41 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 2 | 0.41 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 8 | 0.41 |
| (1,270) | 1:A:101:VAL:HG11 | 1:A:102:ASN:HA | 8 | 0.41 |
| (1,270) | 1:A:101:VAL:HG12 | 1:A:102:ASN:HA | 8 | 0.41 |
| (1,270) | 1:A:101:VAL:HG13 | 1:A:102:ASN:HA | 8 | 0.41 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 6 | 0.41 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG3 | 4 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG2 | 4 | 0.41 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 3 | 0.41 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB1 | 9 | 0.41 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB2 | 9 | 0.41 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB3 | 9 | 0.41 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD3 | 8 | 0.41 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD2 | 8 | 0.41 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 2 | 0.41 |
| (1,2213) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 10 | 0.41 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2081) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 10 | 0.41 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 5 | 0.41 |
| (1,2008) | 1:A:171:LYS:H | 1:A:171:LYS:HA | 10 | 0.41 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 8 | 0.41 |
| (1,1812) | 1:A:152:GLN:HE22 | 1:A:168:PRO:HD3 | 1 | 0.41 |
| (1,1756) | 1:A:148:VAL:H | 1:A:170:PRO:HG3 | 2 | 0.41 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 7 | 0.41 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 7 | 0.41 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 7 | 0.41 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 7 | 0.41 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 7 | 0.41 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 7 | 0.41 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD21 | 3 | 0.41 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD22 | 3 | 0.41 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD23 | 3 | 0.41 |
| (1,1332) | 1:A:95:TRP:H | 1:A:95:TRP:HE3 | 7 | 0.41 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 5 | 0.41 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 5 | 0.41 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 5 | 0.41 |
| (1,99) | 1:A:96:ARG:HB3 | 1:A:164:THR:HB | 5 | 0.4 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 1 | 0.4 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 1 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 1 | 0.4 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 8 | 0.4 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 8 | 0.4 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 8 | 0.4 |
| (1,917) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA2 | 10 | 0.4 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 5 | 0.4 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 5 | 0.4 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 5 | 0.4 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 1 | 0.4 |
| (1,51) | 1:A:95:TRP:HA | 1:A:95:TRP:HB2 | 1 | 0.4 |
| (1,51) | 1:A:95:TRP:HA | 1:A:95:TRP:HB2 | 9 | 0.4 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD2 | 4 | 0.4 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD3 | 4 | 0.4 |
| (1,4262) | 1:B:167:ALA:H | 1:B:166:GLU:HB2 | 4 | 0.4 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 2 | 0.4 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 7 | 0.4 |
| (1,4037) | 1:B:148:VAL:H | 1:B:170:PRO:HG3 | 6 | 0.4 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 7 | 0.4 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 7 | 0.4 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 7 | 0.4 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 10 | 0.4 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 10 | 0.4 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 10 | 0.4 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 10 | 0.4 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 10 | 0.4 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 10 | 0.4 |
| (1,3902) | 1:B:129:ASP:H | 1:B:129:ASP:HB2 | 3 | 0.4 |
| (1,3847) | 1:B:123:LYS:H | 1:B:109:LEU:HB2 | 6 | 0.4 |
| (1,3806) | 1:B:119:GLU:H | 1:B:114:LYS:HB3 | 10 | 0.4 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 3 | 0.4 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 3 | 0.4 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 3 | 0.4 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 8 | 0.4 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 8 | 0.4 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 8 | 0.4 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 8 | 0.4 |
| (1,3612) | 1:B:95:TRP:H | 1:B:95:TRP:HB2 | 2 | 0.4 |
| (1,3612) | 1:B:95:TRP:H | 1:B:95:TRP:HB2 | 3 | 0.4 |
| (1,3601) | 1:B:94:ARG:H | 1:B:92:ALA:HA | 1 | 0.4 |
| (1,3566) | 1:B:168:PRO:HD2 | 1:B:169:MET:HA | 8 | 0.4 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 4 | 0.4 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 8 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 4 | 0.4 |
| (1,3460) | 1:B:157:LEU:HD21 | 1:B:163:LEU:HB3 | 2 | 0.4 |
| (1,3460) | 1:B:157:LEU:HD22 | 1:B:163:LEU:HB3 | 2 | 0.4 |
| (1,3460) | 1:B:157:LEU:HD23 | 1:B:163:LEU:HB3 | 2 | 0.4 |
| (1,3303) | 1:B:148:VAL:HG21 | 1:B:170:PRO:HG2 | 3 | 0.4 |
| (1,3303) | 1:B:148:VAL:HG22 | 1:B:170:PRO:HG2 | 3 | 0.4 |
| (1,3303) | 1:B:148:VAL:HG23 | 1:B:170:PRO:HG2 | 3 | 0.4 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 10 | 0.4 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 10 | 0.4 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 10 | 0.4 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 10 | 0.4 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 10 | 0.4 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 10 | 0.4 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 10 | 0.4 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 10 | 0.4 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 10 | 0.4 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 2 | 0.4 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 2 | 0.4 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 4 | 0.4 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 4 | 0.4 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 2 | 0.4 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 4 | 0.4 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 2 | 0.4 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 2 | 0.4 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 2 | 0.4 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG21 | 10 | 0.4 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG22 | 10 | 0.4 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG23 | 10 | 0.4 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 5 | 0.4 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 5 | 0.4 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 5 | 0.4 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 5 | 0.4 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 5 | 0.4 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 5 | 0.4 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB1 | 7 | 0.4 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB2 | 7 | 0.4 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB3 | 7 | 0.4 |
| (1,2328) | 1:B:94:ARG:HG3 | 1:B:168:PRO:HB3 | 7 | 0.4 |
| (1,2325) | 1:B:94:ARG:HG2 | 1:B:166:GLU:HB2 | 10 | 0.4 |
| (1,2325) | 1:B:94:ARG:HG3 | 1:B:166:GLU:HB2 | 10 | 0.4 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 1 | 0.4 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 10 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 10 | 0.4 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 9 | 0.4 |
| (1,1924) | 1:A:162:THR:H | 1:A:160:GLU:HB2 | 4 | 0.4 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 4 | 0.4 |
| (1,16) | 1:A:93:ASP:HA | 1:A:94:ARG:HD2 | 6 | 0.4 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 4 | 0.4 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 2 | 0.4 |
| (1,1331) | 1:A:95:TRP:H | 1:A:95:TRP:HB2 | 3 | 0.4 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 1 | 0.4 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 1 | 0.4 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 1 | 0.4 |
| (1,1114) | 1:A:155:SER:HB2 | 1:A:163:LEU:HA | 6 | 0.4 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 2 | 0.4 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 2 | 0.4 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 4 | 0.4 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 4 | 0.4 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 4 | 0.4 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 5 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 5 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 5 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 7 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 7 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 7 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 9 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 9 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 9 | 0.39 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 3 | 0.39 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 4 | 0.39 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 4 | 0.39 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 4 | 0.39 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 10 | 0.39 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 10 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 10 | 0.39 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 4 | 0.39 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 7 | 0.39 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG11 | 9 | 0.39 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG12 | 9 | 0.39 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG13 | 9 | 0.39 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD11 | 3 | 0.39 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD12 | 3 | 0.39 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD13 | 3 | 0.39 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD21 | 3 | 0.39 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD22 | 3 | 0.39 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD23 | 3 | 0.39 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 4 | 0.39 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 9 | 0.39 |
| (1,4037) | 1:B:148:VAL:H | 1:B:170:PRO:HG3 | 9 | 0.39 |
| (1,3910) | 1:B:129:ASP:H | 1:B:133:TYR:HB2 | 4 | 0.39 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 2 | 0.39 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 2 | 0.39 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 2 | 0.39 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 4 | 0.39 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 4 | 0.39 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 9 | 0.39 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 9 | 0.39 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 9 | 0.39 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 4 | 0.39 |
| (1,3612) | 1:B:95:TRP:H | 1:B:95:TRP:HB2 | 4 | 0.39 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 8 | 0.39 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 5 | 0.39 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 5 | 0.39 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 5 | 0.39 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 5 | 0.39 |
| (1,3409) | 1:B:155:SER:HB3 | 1:B:157:LEU:HB3 | 10 | 0.39 |
| (1,3409) | 1:B:155:SER:HB2 | 1:B:157:LEU:HB3 | 10 | 0.39 |
| (1,3395) | 1:B:155:SER:HB2 | 1:B:163:LEU:HA | 6 | 0.39 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG21 | 6 | 0.39 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG22 | 6 | 0.39 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG23 | 6 | 0.39 |
| (1,3128) | 1:B:141:LYS:HA | 1:B:141:LYS:HE3 | 9 | 0.39 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 2 | 0.39 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 2 | 0.39 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 6 | 0.39 |
| (1,2935) | 1:B:120:ILE:HD11 | 1:B:140:ARG:HD2 | 6 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2935) | 1:B:120:ILE:HD12 | 1:B:140:ARG:HD2 | 6 | 0.39 |
| (1,2935) | 1:B:120:ILE:HD13 | 1:B:140:ARG:HD2 | 6 | 0.39 |
| (1,2790) | 1:B:114:LYS:HA | 1:B:114:LYS:HB2 | 4 | 0.39 |
| (1,2666) | 1:B:109:LEU:HD21 | 1:B:161:GLY:HA3 | 3 | 0.39 |
| (1,2666) | 1:B:109:LEU:HD22 | 1:B:161:GLY:HA3 | 3 | 0.39 |
| (1,2666) | 1:B:109:LEU:HD23 | 1:B:161:GLY:HA3 | 3 | 0.39 |
| (1,264) | 1:A:100:ASP:HB2 | 1:A:162:THR:HB | 2 | 0.39 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 1 | 0.39 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 9 | 0.39 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD21 | 1 | 0.39 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD22 | 1 | 0.39 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD23 | 1 | 0.39 |
| (1,2332) | 1:B:95:TRP:HA | 1:B:95:TRP:HB2 | 6 | 0.39 |
| (1,2299) | 1:B:93:ASP:HB2 | 1:B:94:ARG:HA | 10 | 0.39 |
| (1,2288) | 1:B:90:HIS:HB2 | 1:B:91:THR:HA | 2 | 0.39 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG2 | 9 | 0.39 |
| (1,2006) | 1:A:171:LYS:H | 1:A:170:PRO:HG3 | 9 | 0.39 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 5 | 0.39 |
| (1,1816) | 1:A:153:VAL:H | 1:A:149:ASP:HB2 | 3 | 0.39 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 2 | 0.39 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 2 | 0.39 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 2 | 0.39 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 9 | 0.39 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 10 | 0.39 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 10 | 0.39 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 10 | 0.39 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 2 | 0.38 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 2 | 0.38 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 2 | 0.38 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 4 | 0.38 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 4 | 0.38 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 4 | 0.38 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 5 | 0.38 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 5 | 0.38 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 5 | 0.38 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD1 | 8 | 0.38 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD2 | 8 | 0.38 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD1 | 8 | 0.38 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD2 | 8 | 0.38 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD1 | 8 | 0.38 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD2 | 8 | 0.38 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 6 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,718) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HB3 | 4 | 0.38 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 2 | 0.38 |
| (1,51) | 1:A:95:TRP:HA | 1:A:95:TRP:HB2 | 6 | 0.38 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 4 | 0.38 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 1 | 0.38 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 1 | 0.38 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 2 | 0.38 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 2 | 0.38 |
| (1,4289) | 1:B:171:LYS:H | 1:B:171:LYS:HA | 5 | 0.38 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 3 | 0.38 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 10 | 0.38 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 3 | 0.38 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 3 | 0.38 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 3 | 0.38 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 4 | 0.38 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 4 | 0.38 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 4 | 0.38 |
| (1,3848) | 1:B:123:LYS:H | 1:B:109:LEU:HG | 8 | 0.38 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 4 | 0.38 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 4 | 0.38 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 4 | 0.38 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 3 | 0.38 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 10 | 0.38 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 3 | 0.38 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 3 | 0.38 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 3 | 0.38 |
| (1,362) | 1:A:109:LEU:HB3 | 1:A:121:THR:HB | 1 | 0.38 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 3 | 0.38 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 4 | 0.38 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD21 | 2 | 0.38 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD22 | 2 | 0.38 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD23 | 2 | 0.38 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 4 | 0.38 |
| (1,3345) | 1:B:152:GLN:HB2 | 1:B:168:PRO:HD3 | 8 | 0.38 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 1 | 0.38 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 2 | 0.38 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 8 | 0.38 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG11 | 9 | 0.38 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG12 | 9 | 0.38 |
| (1,3193) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG13 | 9 | 0.38 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 8 | 0.38 |
| (1,3092) | 1:B:136:ARG:HA | 1:B:136:ARG:HG2 | 8 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3014) | 1:B:126:GLU:HG3 | 1:B:135:SER:HB3 | 6 | 0.38 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 1 | 0.38 |
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 1 | 0.38 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD21 | 5 | 0.38 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD22 | 5 | 0.38 |
| (1,277) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD23 | 5 | 0.38 |
| (1,2651) | 1:B:109:LEU:HD11 | 1:B:122:GLY:HA3 | 9 | 0.38 |
| (1,2651) | 1:B:109:LEU:HD12 | 1:B:122:GLY:HA3 | 9 | 0.38 |
| (1,2651) | 1:B:109:LEU:HD13 | 1:B:122:GLY:HA3 | 9 | 0.38 |
| (1,2617) | 1:B:108:GLU:HA | 1:B:108:GLU:HG2 | 9 | 0.38 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 2 | 0.38 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 5 | 0.38 |
| (1,2568) | 1:B:105:ALA:HA | 1:B:108:GLU:HB3 | 10 | 0.38 |
| (1,2529) | 1:B:99:LEU:HD21 | 1:B:140:ARG:HD2 | 2 | 0.38 |
| (1,2529) | 1:B:99:LEU:HD22 | 1:B:140:ARG:HD2 | 2 | 0.38 |
| (1,2529) | 1:B:99:LEU:HD23 | 1:B:140:ARG:HD2 | 2 | 0.38 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 9 | 0.38 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 10 | 0.38 |
| (1,2149) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2149) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2149) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2149) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2149) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2149) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2017) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2017) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2017) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2017) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2017) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2017) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB2 | 2 | 0.38 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 1 | 0.38 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD2 | 9 | 0.38 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD3 | 9 | 0.38 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 2 | 0.38 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 7 | 0.38 |
| (1,1799) | 1:A:152:GLN:HE21 | 1:A:152:GLN:HB3 | 8 | 0.38 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 6 | 0.38 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 6 | 0.38 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 6 | 0.38 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 6 | 0.38 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 6 | 0.38 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 9 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 9 | 0.38 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 5 | 0.38 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 9 | 0.38 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 6 | 0.38 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 6 | 0.38 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 6 | 0.38 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 6 | 0.38 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 6 | 0.38 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 6 | 0.38 |
| (1,1326) | 1:A:94:ARG:H | 1:A:168:PRO:HA | 1 | 0.38 |
| (1,1288) | 1:A:169:MET:HA | 1:A:169:MET:HG2 | 7 | 0.38 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 5 | 0.38 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 5 | 0.38 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 1 | 0.37 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 1 | 0.37 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 1 | 0.37 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 2 | 0.37 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 2 | 0.37 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 2 | 0.37 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 9 | 0.37 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 9 | 0.37 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 9 | 0.37 |
| (1,928) | 1:A:144:LEU:HD11 | 1:A:145:PRO:HB3 | 10 | 0.37 |
| (1,928) | 1:A:144:LEU:HD12 | 1:A:145:PRO:HB3 | 10 | 0.37 |
| (1,928) | 1:A:144:LEU:HD13 | 1:A:145:PRO:HB3 | 10 | 0.37 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 6 | 0.37 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 7 | 0.37 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 7 | 0.37 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 7 | 0.37 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 6 | 0.37 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 5 | 0.37 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE1 | 5 | 0.37 |
| (1,731) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HE2 | 5 | 0.37 |
| (1,728) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HA | 9 | 0.37 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 9 | 0.37 |
| (1,652) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HB2 | 10 | 0.37 |
| (1,652) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HB2 | 10 | 0.37 |
| (1,652) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HB2 | 10 | 0.37 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 1 | 0.37 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 5 | 0.37 |
| (1,589) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HB | 6 | 0.37 |
| (1,589) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HB | 6 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,589) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HB | 6 | 0.37 |
| (1,51) | 1:A:95:TRP:HA | 1:A:95:TRP:HB2 | 2 | 0.37 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 4 | 0.37 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 3 | 0.37 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 3 | 0.37 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 1 | 0.37 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 1 | 0.37 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 5 | 0.37 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 5 | 0.37 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 5 | 0.37 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE1 | 5 | 0.37 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE2 | 5 | 0.37 |
| (1,3902) | 1:B:129:ASP:H | 1:B:129:ASP:HB2 | 7 | 0.37 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 1 | 0.37 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 1 | 0.37 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 8 | 0.37 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 8 | 0.37 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 8 | 0.37 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 5 | 0.37 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 5 | 0.37 |
| (1,356) | 1:A:109:LEU:HA | 1:A:122:GLY:HA2 | 7 | 0.37 |
| (1,3474) | 1:B:158:SER:HB3 | 1:B:160:GLU:HB3 | 8 | 0.37 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 2 | 0.37 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 10 | 0.37 |
| (1,3409) | 1:B:155:SER:HB3 | 1:B:157:LEU:HB3 | 8 | 0.37 |
| (1,3409) | 1:B:155:SER:HB2 | 1:B:157:LEU:HB3 | 8 | 0.37 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 9 | 0.37 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 6 | 0.37 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 6 | 0.37 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 6 | 0.37 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 8 | 0.37 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 8 | 0.37 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 8 | 0.37 |
| (1,33) | 1:A:94:ARG:HA | 1:A:169:MET:HB2 | 1 | 0.37 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 3 | 0.37 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 4 | 0.37 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD3 | 1 | 0.37 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD2 | 1 | 0.37 |
| (1,3137) | 1:B:141:LYS:HG2 | 1:B:142:TYR:HB3 | 1 | 0.37 |
| (1,3137) | 1:B:141:LYS:HG2 | 1:B:142:TYR:HB3 | 2 | 0.37 |
| (1,3122) | 1:B:140:ARG:HG2 | 1:B:142:TYR:HE1 | 2 | 0.37 |
| (1,3122) | 1:B:140:ARG:HG2 | 1:B:142:TYR:HE2 | 2 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 3 | 0.37 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 5 | 0.37 |
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 8 | 0.37 |
| (1,2783) | 1:B:113:THR:HG21 | 1:B:150:PRO:HB3 | 1 | 0.37 |
| (1,2783) | 1:B:113:THR:HG22 | 1:B:150:PRO:HB3 | 1 | 0.37 |
| (1,2783) | 1:B:113:THR:HG23 | 1:B:150:PRO:HB3 | 1 | 0.37 |
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 8 | 0.37 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 8 | 0.37 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 8 | 0.37 |
| (1,2626) | 1:B:108:GLU:HG2 | 1:B:123:LYS:HE3 | 3 | 0.37 |
| (1,2626) | 1:B:108:GLU:HG2 | 1:B:123:LYS:HE2 | 3 | 0.37 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG21 | 9 | 0.37 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG22 | 9 | 0.37 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG23 | 9 | 0.37 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 10 | 0.37 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 4 | 0.37 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 10 | 0.37 |
| (1,2385) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HA | 10 | 0.37 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 9 | 0.37 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 9 | 0.37 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 9 | 0.37 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 9 | 0.37 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 9 | 0.37 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 9 | 0.37 |
| (1,232) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HG12 | 4 | 0.37 |
| (1,232) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HG12 | 4 | 0.37 |
| (1,232) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HG12 | 4 | 0.37 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 10 | 0.37 |
| (1,2169) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 10 | 0.37 |
| (1,2037) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 10 | 0.37 |
| (1,1998) | 1:A:169:MET:H | 1:A:169:MET:HB2 | 10 | 0.37 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 7 | 0.37 |
| (1,1940) | 1:A:164:THR:H | 1:A:162:THR:HG21 | 2 | 0.37 |
| (1,1940) | 1:A:164:THR:H | 1:A:162:THR:HG22 | 2 | 0.37 |
| (1,1940) | 1:A:164:THR:H | 1:A:162:THR:HG23 | 2 | 0.37 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 4 | 0.37 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 10 | 0.37 |
| (1,184) | 1:A:98:SER:HB2 | 1:A:162:THR:HG21 | 3 | 0.37 |
| (1,184) | 1:A:98:SER:HB2 | 1:A:162:THR:HG22 | 3 | 0.37 |
| (1,184) | 1:A:98:SER:HB2 | 1:A:162:THR:HG23 | 3 | 0.37 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 7 | 0.37 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 7 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 7 | 0.37 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 9 | 0.37 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 9 | 0.37 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 9 | 0.37 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 9 | 0.37 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 9 | 0.37 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 9 | 0.37 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 8 | 0.37 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 8 | 0.37 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 8 | 0.37 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 8 | 0.37 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 8 | 0.37 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 8 | 0.37 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 8 | 0.37 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 8 | 0.37 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 8 | 0.37 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 7 | 0.37 |
| (1,1097) | 1:A:154:SER:HB3 | 1:A:155:SER:HA | 1 | 0.37 |
| (1,990) | 1:A:148:VAL:HA | 1:A:169:MET:HB2 | 6 | 0.36 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 1 | 0.36 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 1 | 0.36 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 1 | 0.36 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 1 | 0.36 |
| (1,847) | 1:A:141:LYS:HA | 1:A:141:LYS:HE3 | 7 | 0.36 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD1 | 1 | 0.36 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD2 | 1 | 0.36 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD1 | 1 | 0.36 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD2 | 1 | 0.36 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD1 | 1 | 0.36 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD2 | 1 | 0.36 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 4 | 0.36 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 2 | 0.36 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 2 | 0.36 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 2 | 0.36 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 9 | 0.36 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 9 | 0.36 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 9 | 0.36 |
| (1,4293) | 1:B:172:LEU:H | 1:B:171:LYS:HA | 2 | 0.36 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB1 | 7 | 0.36 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB2 | 7 | 0.36 |
| (1,4274) | 1:B:169:MET:H | 1:B:167:ALA:HB3 | 7 | 0.36 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 3 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 9 | 0.36 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 9 | 0.36 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 9 | 0.36 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 6 | 0.36 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 9 | 0.36 |
| (1,3436) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HA | 9 | 0.36 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 1 | 0.36 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 2 | 0.36 |
| (1,336) | 1:A:108:GLU:HA | 1:A:108:GLU:HG2 | 2 | 0.36 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 2 | 0.36 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 5 | 0.36 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 9 | 0.36 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 6 | 0.36 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 6 | 0.36 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 6 | 0.36 |
| (1,3139) | 1:B:141:LYS:HG3 | 1:B:141:LYS:HE2 | 10 | 0.36 |
| (1,3060) | 1:B:131:HIS:HA | 1:B:131:HIS:HE1 | 9 | 0.36 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 6 | 0.36 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 7 | 0.36 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 3 | 0.36 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 6 | 0.36 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 6 | 0.36 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 6 | 0.36 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 3 | 0.36 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 3 | 0.36 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 3 | 0.36 |
| (1,2738) | 1:B:112:LYS:HB2 | 1:B:120:ILE:HA | 8 | 0.36 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 9 | 0.36 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 4 | 0.36 |
| (1,2637) | 1:B:109:LEU:HA | 1:B:122:GLY:HA2 | 8 | 0.36 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 3 | 0.36 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 3 | 0.36 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 3 | 0.36 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 3 | 0.36 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 3 | 0.36 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 3 | 0.36 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG21 | 6 | 0.36 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG22 | 6 | 0.36 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG23 | 6 | 0.36 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 8 | 0.36 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 3 | 0.36 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 3 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 3 | 0.36 |
| (1,2314) | 1:B:94:ARG:HA | 1:B:169:MET:HB2 | 8 | 0.36 |
| (1,1974) | 1:A:167:ALA:H | 1:A:95:TRP:HB3 | 5 | 0.36 |
| (1,1916) | 1:A:162:THR:H | 1:A:102:ASN:HB3 | 3 | 0.36 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 1 | 0.36 |
| (1,1642) | 1:A:132:GLY:H | 1:A:129:ASP:HB2 | 3 | 0.36 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 10 | 0.36 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 10 | 0.36 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 10 | 0.36 |
| (1,1332) | 1:A:95:TRP:H | 1:A:95:TRP:HE3 | 4 | 0.36 |
| (1,1321) | 1:A:94:ARG:H | 1:A:93:ASP:HA | 8 | 0.36 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG21 | 10 | 0.36 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG22 | 10 | 0.36 |
| (1,1319) | 1:A:94:ARG:H | 1:A:91:THR:HG23 | 10 | 0.36 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 3 | 0.36 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 3 | 0.36 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 3 | 0.36 |
| (1,1097) | 1:A:154:SER:HB3 | 1:A:155:SER:HA | 9 | 0.36 |
| (1,1085) | 1:A:153:VAL:HG11 | 1:A:155:SER:HB3 | 6 | 0.36 |
| (1,1085) | 1:A:153:VAL:HG12 | 1:A:155:SER:HB3 | 6 | 0.36 |
| (1,1085) | 1:A:153:VAL:HG13 | 1:A:155:SER:HB3 | 6 | 0.36 |
| (1,1085) | 1:A:153:VAL:HG21 | 1:A:155:SER:HB3 | 6 | 0.36 |
| (1,1085) | 1:A:153:VAL:HG22 | 1:A:155:SER:HB3 | 6 | 0.36 |
| (1,1085) | 1:A:153:VAL:HG23 | 1:A:155:SER:HB3 | 6 | 0.36 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 4 | 0.36 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 4 | 0.36 |
| (1,9) | 1:A:90:HIS:HB3 | 1:A:91:THR:HA | 2 | 0.35 |
| (1,858) | 1:A:141:LYS:HG3 | 1:A:141:LYS:HE2 | 10 | 0.35 |
| (1,841) | 1:A:140:ARG:HG2 | 1:A:142:TYR:HE1 | 4 | 0.35 |
| (1,841) | 1:A:140:ARG:HG2 | 1:A:142:TYR:HE2 | 4 | 0.35 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 3 | 0.35 |
| (1,718) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HB3 | 1 | 0.35 |
| (1,718) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HB3 | 5 | 0.35 |
| (1,654) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HD2 | 9 | 0.35 |
| (1,654) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HD2 | 9 | 0.35 |
| (1,654) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HD2 | 9 | 0.35 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 10 | 0.35 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 10 | 0.35 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 10 | 0.35 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 9 | 0.35 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 8 | 0.35 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 8 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,457) | 1:A:112:LYS:HB2 | 1:A:120:ILE:HA | 3 | 0.35 |
| (1,4084) | 1:B:152:GLN:HE21 | 1:B:168:PRO:HD2 | 10 | 0.35 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 9 | 0.35 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 4 | 0.35 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 4 | 0.35 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 4 | 0.35 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 4 | 0.35 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 4 | 0.35 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 4 | 0.35 |
| (1,3915) | 1:B:131:HIS:H | 1:B:129:ASP:HB3 | 2 | 0.35 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 5 | 0.35 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 5 | 0.35 |
| (1,3847) | 1:B:123:LYS:H | 1:B:109:LEU:HB2 | 9 | 0.35 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 10 | 0.35 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 10 | 0.35 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 10 | 0.35 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 10 | 0.35 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 10 | 0.35 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 10 | 0.35 |
| (1,3474) | 1:B:158:SER:HB3 | 1:B:160:GLU:HB3 | 3 | 0.35 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 6 | 0.35 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 5 | 0.35 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 4 | 0.35 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 4 | 0.35 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 4 | 0.35 |
| (1,3304) | 1:B:149:ASP:HA | 1:B:149:ASP:HB3 | 5 | 0.35 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG11 | 1 | 0.35 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG12 | 1 | 0.35 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG13 | 1 | 0.35 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG11 | 1 | 0.35 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG12 | 1 | 0.35 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG13 | 1 | 0.35 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 3 | 0.35 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 3 | 0.35 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 3 | 0.35 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 10 | 0.35 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 10 | 0.35 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 10 | 0.35 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 10 | 0.35 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 10 | 0.35 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 10 | 0.35 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 6 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 8 | 0.35 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 10 | 0.35 |
| (1,2971) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HB2 | 1 | 0.35 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 10 | 0.35 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 10 | 0.35 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 10 | 0.35 |
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 5 | 0.35 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 5 | 0.35 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 9 | 0.35 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 6 | 0.35 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 6 | 0.35 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 6 | 0.35 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 5 | 0.35 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 2 | 0.35 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 10 | 0.35 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 10 | 0.35 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 10 | 0.35 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 10 | 0.35 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 10 | 0.35 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 10 | 0.35 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 6 | 0.35 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB1 | 6 | 0.35 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB2 | 6 | 0.35 |
| (1,2344) | 1:B:95:TRP:HB2 | 1:B:167:ALA:HB3 | 6 | 0.35 |
| (1,2299) | 1:B:93:ASP:HB2 | 1:B:94:ARG:HA | 4 | 0.35 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 4 | 0.35 |
| (1,2286) | 1:B:90:HIS:HA | 1:B:91:THR:HA | 8 | 0.35 |
| (1,2213) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 8 | 0.35 |
| (1,2081) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 8 | 0.35 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 9 | 0.35 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 9 | 0.35 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 3 | 0.35 |
| (1,1816) | 1:A:153:VAL:H | 1:A:149:ASP:HB2 | 9 | 0.35 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 10 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 3 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 3 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 3 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 3 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 3 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 3 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 5 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 5 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 5 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 5 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 5 | 0.35 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 5 | 0.35 |
| (1,1423) | 1:A:108:GLU:H | 1:A:123:LYS:HG2 | 3 | 0.35 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 4 | 0.35 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 5 | 0.35 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 1 | 0.35 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 1 | 0.35 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 1 | 0.35 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 1 | 0.35 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 1 | 0.35 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 1 | 0.35 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 5 | 0.35 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 5 | 0.35 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 5 | 0.35 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 9 | 0.35 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 9 | 0.35 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 9 | 0.35 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 9 | 0.35 |
| (1,1193) | 1:A:158:SER:HB3 | 1:A:160:GLU:HB3 | 8 | 0.35 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 6 | 0.35 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 6 | 0.35 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 6 | 0.35 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 8 | 0.35 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 10 | 0.35 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 1 | 0.35 |
| (1,99) | 1:A:96:ARG:HB3 | 1:A:164:THR:HB | 9 | 0.34 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG3 | 4 | 0.34 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG2 | 4 | 0.34 |
| (1,847) | 1:A:141:LYS:HA | 1:A:141:LYS:HE3 | 1 | 0.34 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 2 | 0.34 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 1 | 0.34 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 1 | 0.34 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 1 | 0.34 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 1 | 0.34 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 8 | 0.34 |
| (1,722) | 1:A:126:GLU:HG2 | 1:A:135:SER:HA | 2 | 0.34 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 1 | 0.34 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 1 | 0.34 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 3 | 0.34 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 3 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 4 | 0.34 |
| (1,688) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB3 | 9 | 0.34 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD1 | 4 | 0.34 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD2 | 4 | 0.34 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD1 | 4 | 0.34 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD2 | 4 | 0.34 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD1 | 4 | 0.34 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD2 | 4 | 0.34 |
| (1,435) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG13 | 10 | 0.34 |
| (1,435) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG13 | 10 | 0.34 |
| (1,435) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG13 | 10 | 0.34 |
| (1,435) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG13 | 10 | 0.34 |
| (1,435) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG13 | 10 | 0.34 |
| (1,435) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG13 | 10 | 0.34 |
| (1,4182) | 1:B:161:GLY:H | 1:B:102:ASN:HB2 | 3 | 0.34 |
| (1,4051) | 1:B:151:THR:H | 1:B:149:ASP:HB2 | 5 | 0.34 |
| (1,4024) | 1:B:148:VAL:H | 1:B:146:PRO:HB3 | 4 | 0.34 |
| (1,3902) | 1:B:129:ASP:H | 1:B:129:ASP:HB2 | 2 | 0.34 |
| (1,3833) | 1:B:121:THR:H | 1:B:120:ILE:HG12 | 9 | 0.34 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD21 | 9 | 0.34 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD22 | 9 | 0.34 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD23 | 9 | 0.34 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 1 | 0.34 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 1 | 0.34 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 1 | 0.34 |
| (1,3491) | 1:B:160:GLU:HB2 | 1:B:162:THR:HB | 6 | 0.34 |
| (1,3460) | 1:B:157:LEU:HD21 | 1:B:163:LEU:HB3 | 3 | 0.34 |
| (1,3460) | 1:B:157:LEU:HD22 | 1:B:163:LEU:HB3 | 3 | 0.34 |
| (1,3460) | 1:B:157:LEU:HD23 | 1:B:163:LEU:HB3 | 3 | 0.34 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 9 | 0.34 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 9 | 0.34 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 9 | 0.34 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 2 | 0.34 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 6 | 0.34 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 6 | 0.34 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 7 | 0.34 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 7 | 0.34 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 7 | 0.34 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 7 | 0.34 |
| (1,3302) | 1:B:148:VAL:HG21 | 1:B:169:MET:HB3 | 1 | 0.34 |
| (1,3302) | 1:B:148:VAL:HG22 | 1:B:169:MET:HB3 | 1 | 0.34 |
| (1,3302) | 1:B:148:VAL:HG23 | 1:B:169:MET:HB3 | 1 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 4 | 0.34 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 8 | 0.34 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 10 | 0.34 |
| (1,2971) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HB2 | 4 | 0.34 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 10 | 0.34 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 10 | 0.34 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 10 | 0.34 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD11 | 5 | 0.34 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD12 | 5 | 0.34 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD13 | 5 | 0.34 |
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 10 | 0.34 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 10 | 0.34 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 10 | 0.34 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 10 | 0.34 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 10 | 0.34 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD11 | 9 | 0.34 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD12 | 9 | 0.34 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD13 | 9 | 0.34 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB1 | 3 | 0.34 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB2 | 3 | 0.34 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB3 | 3 | 0.34 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 7 | 0.34 |
| (1,2200) | 1:B:134:ILE:HG21 | 1:A:140:ARG:HD3 | 4 | 0.34 |
| (1,2200) | 1:B:134:ILE:HG22 | 1:A:140:ARG:HD3 | 4 | 0.34 |
| (1,2200) | 1:B:134:ILE:HG23 | 1:A:140:ARG:HD3 | 4 | 0.34 |
| (1,2169) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 6 | 0.34 |
| (1,2169) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 7 | 0.34 |
| (1,2068) | 1:B:134:ILE:HG21 | 1:A:140:ARG:HD3 | 4 | 0.34 |
| (1,2068) | 1:B:134:ILE:HG22 | 1:A:140:ARG:HD3 | 4 | 0.34 |
| (1,2068) | 1:B:134:ILE:HG23 | 1:A:140:ARG:HD3 | 4 | 0.34 |
| (1,2037) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 6 | 0.34 |
| (1,2037) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 7 | 0.34 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD2 | 7 | 0.34 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD3 | 7 | 0.34 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 1 | 0.34 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 4 | 0.34 |
| (1,1654) | 1:A:134:ILE:H | 1:A:127:ARG:HB2 | 6 | 0.34 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD1 | 5 | 0.34 |
| (1,1630) | 1:A:129:ASP:H | 1:A:133:TYR:HD2 | 5 | 0.34 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 7 | 0.34 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 10 | 0.34 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD11 | 3 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD12 | 3 | 0.34 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD13 | 3 | 0.34 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 4 | 0.34 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 4 | 0.34 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 4 | 0.34 |
| (1,1321) | 1:A:94:ARG:H | 1:A:93:ASP:HA | 5 | 0.34 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 2 | 0.34 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 2 | 0.34 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 2 | 0.34 |
| (1,1193) | 1:A:158:SER:HB3 | 1:A:160:GLU:HB3 | 6 | 0.34 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 4 | 0.34 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 8 | 0.34 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 2 | 0.34 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 4 | 0.34 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 5 | 0.34 |
| (1,1065) | 1:A:152:GLN:HB2 | 1:A:169:MET:HA | 9 | 0.34 |
| (1,102) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HB3 | 2 | 0.34 |
| (1,99) | 1:A:96:ARG:HB3 | 1:A:164:THR:HB | 2 | 0.33 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD1 | 3 | 0.33 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD2 | 3 | 0.33 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD1 | 3 | 0.33 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD2 | 3 | 0.33 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD1 | 3 | 0.33 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD2 | 3 | 0.33 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD1 | 4 | 0.33 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD2 | 4 | 0.33 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD1 | 4 | 0.33 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD2 | 4 | 0.33 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD1 | 4 | 0.33 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD2 | 4 | 0.33 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 9 | 0.33 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE1 | 7 | 0.33 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE2 | 7 | 0.33 |
| (1,707) | 1:A:126:GLU:HA | 1:A:133:TYR:HB3 | 2 | 0.33 |
| (1,703) | 1:A:125:GLU:HA | 1:A:135:SER:HB2 | 4 | 0.33 |
| (1,612) | 1:A:119:GLU:HA | 1:A:141:LYS:HE3 | 7 | 0.33 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 4 | 0.33 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 4 | 0.33 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 4 | 0.33 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 4 | 0.33 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 4 | 0.33 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 4 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,528) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HB | 7 | 0.33 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 2 | 0.33 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 4 | 0.33 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG2 | 6 | 0.33 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG3 | 6 | 0.33 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG21 | 9 | 0.33 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG22 | 9 | 0.33 |
| (1,4221) | 1:B:164:THR:H | 1:B:162:THR:HG23 | 9 | 0.33 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 4 | 0.33 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 9 | 0.33 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 2 | 0.33 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 1 | 0.33 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 1 | 0.33 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 1 | 0.33 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 6 | 0.33 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 6 | 0.33 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 6 | 0.33 |
| (1,3935) | 1:B:134:ILE:H | 1:B:127:ARG:HB2 | 2 | 0.33 |
| (1,3907) | 1:B:129:ASP:H | 1:B:132:GLY:HA3 | 8 | 0.33 |
| (1,3847) | 1:B:123:LYS:H | 1:B:109:LEU:HB2 | 2 | 0.33 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 9 | 0.33 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 9 | 0.33 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 9 | 0.33 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 5 | 0.33 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 5 | 0.33 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 5 | 0.33 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 3 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG11 | 7 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG12 | 7 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG13 | 7 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG11 | 7 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG12 | 7 | 0.33 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG13 | 7 | 0.33 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 1 | 0.33 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 1 | 0.33 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 1 | 0.33 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD3 | 10 | 0.33 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD2 | 10 | 0.33 |
| (1,3060) | 1:B:131:HIS:HA | 1:B:131:HIS:HE1 | 3 | 0.33 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 7 | 0.33 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 7 | 0.33 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 7 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 8 | 0.33 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 8 | 0.33 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 8 | 0.33 |
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 3 | 0.33 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 3 | 0.33 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 3 | 0.33 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 3 | 0.33 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 3 | 0.33 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 8 | 0.33 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 8 | 0.33 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 8 | 0.33 |
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 2 | 0.33 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 2 | 0.33 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 2 | 0.33 |
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 10 | 0.33 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 10 | 0.33 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 10 | 0.33 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD11 | 10 | 0.33 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD12 | 10 | 0.33 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD13 | 10 | 0.33 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 10 | 0.33 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 9 | 0.33 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 7 | 0.33 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 7 | 0.33 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 7 | 0.33 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 5 | 0.33 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 5 | 0.33 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 5 | 0.33 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 5 | 0.33 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 5 | 0.33 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 5 | 0.33 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 7 | 0.33 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 10 | 0.33 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 10 | 0.33 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 10 | 0.33 |
| (1,2568) | 1:B:105:ALA:HA | 1:B:108:GLU:HB3 | 3 | 0.33 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 1 | 0.33 |
| (1,2299) | 1:B:93:ASP:HB2 | 1:B:94:ARG:HA | 1 | 0.33 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 8 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 5 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2152) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2152) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 5 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2020) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 9 | 0.33 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 3 | 0.33 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 2 | 0.33 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 2 | 0.33 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 1 | 0.33 |
| (1,1847) | 1:A:155:SER:H | 1:A:154:SER:HB2 | 9 | 0.33 |
| (1,1634) | 1:A:131:HIS:H | 1:A:129:ASP:HB3 | 3 | 0.33 |
| (1,1621) | 1:A:129:ASP:H | 1:A:129:ASP:HB2 | 6 | 0.33 |
| (1,1587) | 1:A:126:GLU:H | 1:A:125:GLU:HG2 | 2 | 0.33 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 4 | 0.33 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 1 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1179) | 1:A:157:LEU:HD21 | 1:A:163:LEU:HB3 | 8 | 0.33 |
| (1,1179) | 1:A:157:LEU:HD22 | 1:A:163:LEU:HB3 | 8 | 0.33 |
| (1,1179) | 1:A:157:LEU:HD23 | 1:A:163:LEU:HB3 | 8 | 0.33 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 3 | 0.33 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 3 | 0.33 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 2 | 0.33 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 9 | 0.33 |
| (1,102) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HB3 | 9 | 0.33 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 8 | 0.32 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 8 | 0.32 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 8 | 0.32 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 4 | 0.32 |
| (1,835) | 1:A:139:THR:HG21 | 1:A:141:LYS:HE2 | 9 | 0.32 |
| (1,835) | 1:A:139:THR:HG22 | 1:A:141:LYS:HE2 | 9 | 0.32 |
| (1,835) | 1:A:139:THR:HG23 | 1:A:141:LYS:HE2 | 9 | 0.32 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 5 | 0.32 |
| (1,7) | 1:A:90:HIS:HB2 | 1:A:91:THR:HA | 6 | 0.32 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 10 | 0.32 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 10 | 0.32 |
| (1,693) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB3 | 10 | 0.32 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD1 | 9 | 0.32 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD2 | 9 | 0.32 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD1 | 9 | 0.32 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD2 | 9 | 0.32 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD1 | 9 | 0.32 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD2 | 9 | 0.32 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 3 | 0.32 |
| (1,635) | 1:A:120:ILE:HB | 1:A:140:ARG:HD2 | 10 | 0.32 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 1 | 0.32 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD11 | 4 | 0.32 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD12 | 4 | 0.32 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD13 | 4 | 0.32 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD21 | 4 | 0.32 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD22 | 4 | 0.32 |
| (1,4295) | 1:B:172:LEU:H | 1:B:172:LEU:HD23 | 4 | 0.32 |
| (1,4281) | 1:B:169:MET:H | 1:B:169:MET:HG3 | 9 | 0.32 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB1 | 10 | 0.32 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB2 | 10 | 0.32 |
| (1,4268) | 1:B:169:MET:H | 1:B:92:ALA:HB3 | 10 | 0.32 |
| (1,4255) | 1:B:167:ALA:H | 1:B:95:TRP:HB3 | 1 | 0.32 |
| (1,4205) | 1:B:162:THR:H | 1:B:160:GLU:HB2 | 9 | 0.32 |
| (1,42) | 1:A:94:ARG:HB3 | 1:A:168:PRO:HA | 1 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4197) | 1:B:162:THR:H | 1:B:102:ASN:HB3 | 6 | 0.32 |
| (1,4128) | 1:B:155:SER:H | 1:B:154:SER:HB2 | 7 | 0.32 |
| (1,3955) | 1:B:137:CYS:H | 1:B:136:ARG:HB3 | 9 | 0.32 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 10 | 0.32 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 10 | 0.32 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 9 | 0.32 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 9 | 0.32 |
| (1,3847) | 1:B:123:LYS:H | 1:B:109:LEU:HB2 | 3 | 0.32 |
| (1,3847) | 1:B:123:LYS:H | 1:B:109:LEU:HB2 | 5 | 0.32 |
| (1,3827) | 1:B:120:ILE:H | 1:B:142:TYR:H | 2 | 0.32 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 4 | 0.32 |
| (1,3825) | 1:B:120:ILE:H | 1:B:140:ARG:HG2 | 2 | 0.32 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 1 | 0.32 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD21 | 1 | 0.32 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD22 | 1 | 0.32 |
| (1,3653) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD23 | 1 | 0.32 |
| (1,3613) | 1:B:95:TRP:H | 1:B:95:TRP:HE3 | 8 | 0.32 |
| (1,3604) | 1:B:94:ARG:H | 1:B:93:ASP:HB3 | 1 | 0.32 |
| (1,3602) | 1:B:94:ARG:H | 1:B:93:ASP:HA | 4 | 0.32 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 6 | 0.32 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 1 | 0.32 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 7 | 0.32 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 7 | 0.32 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 7 | 0.32 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 1 | 0.32 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 6 | 0.32 |
| (1,3096) | 1:B:136:ARG:HG3 | 1:B:138:PHE:HA | 9 | 0.32 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 10 | 0.32 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 10 | 0.32 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 1 | 0.32 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 3 | 0.32 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 3 | 0.32 |
| (1,2929) | 1:B:120:ILE:HG21 | 1:B:139:THR:HA | 10 | 0.32 |
| (1,2929) | 1:B:120:ILE:HG22 | 1:B:139:THR:HA | 10 | 0.32 |
| (1,2929) | 1:B:120:ILE:HG23 | 1:B:139:THR:HA | 10 | 0.32 |
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 7 | 0.32 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 2 | 0.32 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 2 | 0.32 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 2 | 0.32 |
| (1,2715) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG12 | 6 | 0.32 |
| (1,2715) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG12 | 6 | 0.32 |
| (1,2715) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG12 | 6 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2715) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG12 | 6 | 0.32 |
| (1,2715) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG12 | 6 | 0.32 |
| (1,2715) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG12 | 6 | 0.32 |
| (1,2617) | 1:B:108:GLU:HA | 1:B:108:GLU:HG2 | 5 | 0.32 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 4 | 0.32 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 7 | 0.32 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 3 | 0.32 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 3 | 0.32 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 3 | 0.32 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG3 | 5 | 0.32 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG2 | 5 | 0.32 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 1 | 0.32 |
| (1,2282) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HA | 1 | 0.32 |
| (1,2282) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HA | 1 | 0.32 |
| (1,2282) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HA | 1 | 0.32 |
| (1,1974) | 1:A:167:ALA:H | 1:A:95:TRP:HB3 | 7 | 0.32 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG21 | 2 | 0.32 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG22 | 2 | 0.32 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG23 | 2 | 0.32 |
| (1,1794) | 1:A:152:GLN:H | 1:A:168:PRO:HD3 | 1 | 0.32 |
| (1,1756) | 1:A:148:VAL:H | 1:A:170:PRO:HG3 | 9 | 0.32 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 5 | 0.32 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 5 | 0.32 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 5 | 0.32 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 5 | 0.32 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 5 | 0.32 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 5 | 0.32 |
| (1,1664) | 1:A:135:SER:H | 1:A:134:ILE:HG13 | 1 | 0.32 |
| (1,1621) | 1:A:129:ASP:H | 1:A:129:ASP:HB2 | 3 | 0.32 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 1 | 0.32 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 1 | 0.32 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 3 | 0.32 |
| (1,1322) | 1:A:94:ARG:H | 1:A:93:ASP:HB2 | 7 | 0.32 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 3 | 0.32 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 7 | 0.32 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 6 | 0.32 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG11 | 10 | 0.31 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG12 | 10 | 0.31 |
| (1,974) | 1:A:147:GLY:HA2 | 1:A:148:VAL:HG13 | 10 | 0.31 |
| (1,930) | 1:A:144:LEU:HD11 | 1:A:148:VAL:HA | 10 | 0.31 |
| (1,930) | 1:A:144:LEU:HD12 | 1:A:148:VAL:HA | 10 | 0.31 |
| (1,930) | 1:A:144:LEU:HD13 | 1:A:148:VAL:HA | 10 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 10 | 0.31 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 10 | 0.31 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 10 | 0.31 |
| (1,827) | 1:A:139:THR:HA | 1:A:140:ARG:HG2 | 9 | 0.31 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 4 | 0.31 |
| (1,746) | 1:A:128:GLN:HA | 1:A:128:GLN:HG3 | 2 | 0.31 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 2 | 0.31 |
| (1,648) | 1:A:120:ILE:HG21 | 1:A:139:THR:HA | 1 | 0.31 |
| (1,648) | 1:A:120:ILE:HG22 | 1:A:139:THR:HA | 1 | 0.31 |
| (1,648) | 1:A:120:ILE:HG23 | 1:A:139:THR:HA | 1 | 0.31 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG21 | 1 | 0.31 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG22 | 1 | 0.31 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG23 | 1 | 0.31 |
| (1,528) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HB | 2 | 0.31 |
| (1,4205) | 1:B:162:THR:H | 1:B:160:GLU:HB2 | 10 | 0.31 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 4 | 0.31 |
| (1,4128) | 1:B:155:SER:H | 1:B:154:SER:HB2 | 4 | 0.31 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 4 | 0.31 |
| (1,4065) | 1:B:152:GLN:H | 1:B:149:ASP:HB3 | 3 | 0.31 |
| (1,3935) | 1:B:134:ILE:H | 1:B:127:ARG:HB2 | 3 | 0.31 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 2 | 0.31 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 2 | 0.31 |
| (1,3862) | 1:B:125:GLU:H | 1:B:108:GLU:HG3 | 4 | 0.31 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 1 | 0.31 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 5 | 0.31 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 7 | 0.31 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 4 | 0.31 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 8 | 0.31 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 5 | 0.31 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 10 | 0.31 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG11 | 2 | 0.31 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG12 | 2 | 0.31 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG13 | 2 | 0.31 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG11 | 2 | 0.31 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG12 | 2 | 0.31 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG13 | 2 | 0.31 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 3 | 0.31 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 5 | 0.31 |
| (1,3209) | 1:B:144:LEU:HD11 | 1:B:145:PRO:HB3 | 3 | 0.31 |
| (1,3209) | 1:B:144:LEU:HD12 | 1:B:145:PRO:HB3 | 3 | 0.31 |
| (1,3209) | 1:B:144:LEU:HD13 | 1:B:145:PRO:HB3 | 3 | 0.31 |
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 3 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,320) | 1:A:106:PRO:HB2 | 1:A:106:PRO:HD3 | 10 | 0.31 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 4 | 0.31 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 4 | 0.31 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 4 | 0.31 |
| (1,3139) | 1:B:141:LYS:HG3 | 1:B:141:LYS:HE2 | 1 | 0.31 |
| (1,3139) | 1:B:141:LYS:HG3 | 1:B:141:LYS:HE2 | 2 | 0.31 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 1 | 0.31 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 5 | 0.31 |
| (1,3018) | 1:B:127:ARG:HA | 1:B:127:ARG:HD3 | 1 | 0.31 |
| (1,3018) | 1:B:127:ARG:HA | 1:B:127:ARG:HD3 | 2 | 0.31 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE1 | 10 | 0.31 |
| (1,3012) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HE2 | 10 | 0.31 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 1 | 0.31 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 1 | 0.31 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG21 | 4 | 0.31 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG22 | 4 | 0.31 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG23 | 4 | 0.31 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG21 | 8 | 0.31 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG22 | 8 | 0.31 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG23 | 8 | 0.31 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 5 | 0.31 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 5 | 0.31 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 5 | 0.31 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG11 | 10 | 0.31 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG12 | 10 | 0.31 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG13 | 10 | 0.31 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 3 | 0.31 |
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 5 | 0.31 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 5 | 0.31 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 5 | 0.31 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD11 | 1 | 0.31 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD12 | 1 | 0.31 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD13 | 1 | 0.31 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 7 | 0.31 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 7 | 0.31 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 7 | 0.31 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 7 | 0.31 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 7 | 0.31 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 7 | 0.31 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 9 | 0.31 |
| (1,2601) | 1:B:106:PRO:HB2 | 1:B:106:PRO:HD3 | 3 | 0.31 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 1 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 1 | 0.31 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 1 | 0.31 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG3 | 10 | 0.31 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG2 | 10 | 0.31 |
| (1,2377) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HB2 | 5 | 0.31 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 6 | 0.31 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 6 | 0.31 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 6 | 0.31 |
| (1,2330) | 1:B:94:ARG:HD3 | 1:B:168:PRO:HA | 8 | 0.31 |
| (1,2329) | 1:B:94:ARG:HD2 | 1:B:168:PRO:HA | 7 | 0.31 |
| (1,1998) | 1:A:169:MET:H | 1:A:169:MET:HB2 | 5 | 0.31 |
| (1,1902) | 1:A:161:GLY:H | 1:A:102:ASN:HB3 | 2 | 0.31 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 9 | 0.31 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 9 | 0.31 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 9 | 0.31 |
| (1,1640) | 1:A:132:GLY:H | 1:A:128:GLN:HG2 | 1 | 0.31 |
| (1,1634) | 1:A:131:HIS:H | 1:A:129:ASP:HB3 | 7 | 0.31 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 5 | 0.31 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 5 | 0.31 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 3 | 0.31 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 8 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 1 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 1 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 1 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 1 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 1 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 1 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 6 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 6 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 6 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 6 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 6 | 0.31 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 6 | 0.31 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 1 | 0.31 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 1 | 0.31 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 1 | 0.31 |
| (1,1323) | 1:A:94:ARG:H | 1:A:93:ASP:HB3 | 4 | 0.31 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 6 | 0.31 |
| (1,1163) | 1:A:157:LEU:HG | 1:A:161:GLY:HA3 | 8 | 0.31 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 5 | 0.31 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 2 | 0.31 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 2 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 2 | 0.31 |
| (1,920) | 1:A:144:LEU:HB3 | 1:A:148:VAL:HG21 | 6 | 0.3 |
| (1,920) | 1:A:144:LEU:HB3 | 1:A:148:VAL:HG22 | 6 | 0.3 |
| (1,920) | 1:A:144:LEU:HB3 | 1:A:148:VAL:HG23 | 6 | 0.3 |
| (1,777) | 1:A:131:HIS:HA | 1:A:131:HIS:HB3 | 2 | 0.3 |
| (1,723) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB2 | 10 | 0.3 |
| (1,699) | 1:A:125:GLU:HA | 1:A:125:GLU:HG2 | 9 | 0.3 |
| (1,690) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HB2 | 6 | 0.3 |
| (1,684) | 1:A:123:LYS:HA | 1:A:135:SER:HB3 | 4 | 0.3 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 8 | 0.3 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 8 | 0.3 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 8 | 0.3 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 8 | 0.3 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 1 | 0.3 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 1 | 0.3 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 1 | 0.3 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 7 | 0.3 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 7 | 0.3 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 7 | 0.3 |
| (1,5) | 1:A:90:HIS:HA | 1:A:91:THR:HA | 6 | 0.3 |
| (1,435) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG13 | 8 | 0.3 |
| (1,435) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG13 | 8 | 0.3 |
| (1,435) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG13 | 8 | 0.3 |
| (1,435) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG13 | 8 | 0.3 |
| (1,435) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG13 | 8 | 0.3 |
| (1,435) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG13 | 8 | 0.3 |
| (1,4280) | 1:B:169:MET:H | 1:B:169:MET:HB3 | 8 | 0.3 |
| (1,4205) | 1:B:162:THR:H | 1:B:160:GLU:HB2 | 2 | 0.3 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 1 | 0.3 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 1 | 0.3 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 1 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 1 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 1 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 1 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 1 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 1 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 1 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 6 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 6 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 6 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 6 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 6 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 6 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 9 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 9 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 9 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 9 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 9 | 0.3 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 9 | 0.3 |
| (1,3915) | 1:B:131:HIS:H | 1:B:129:ASP:HB3 | 7 | 0.3 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 2 | 0.3 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 2 | 0.3 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 2 | 0.3 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD11 | 8 | 0.3 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD12 | 8 | 0.3 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD13 | 8 | 0.3 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD21 | 8 | 0.3 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD22 | 8 | 0.3 |
| (1,3713) | 1:B:109:LEU:H | 1:B:157:LEU:HD23 | 8 | 0.3 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 8 | 0.3 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD22 | 6 | 0.3 |
| (1,3648) | 1:B:102:ASN:H | 1:B:102:ASN:HD21 | 6 | 0.3 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 9 | 0.3 |
| (1,3491) | 1:B:160:GLU:HB2 | 1:B:162:THR:HB | 7 | 0.3 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 3 | 0.3 |
| (1,3409) | 1:B:155:SER:HB3 | 1:B:157:LEU:HB3 | 2 | 0.3 |
| (1,3409) | 1:B:155:SER:HB2 | 1:B:157:LEU:HB3 | 2 | 0.3 |
| (1,3400) | 1:B:155:SER:HB2 | 1:B:165:VAL:HA | 5 | 0.3 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 7 | 0.3 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 6 | 0.3 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 6 | 0.3 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 6 | 0.3 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 6 | 0.3 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 6 | 0.3 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 6 | 0.3 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 7 | 0.3 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 10 | 0.3 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 7 | 0.3 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 2 | 0.3 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 10 | 0.3 |
| (1,3018) | 1:B:127:ARG:HA | 1:B:127:ARG:HD3 | 7 | 0.3 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG21 | 1 | 0.3 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG22 | 1 | 0.3 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG23 | 1 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2891) | 1:B:119:GLU:HA | 1:B:141:LYS:HD3 | 6 | 0.3 |
| (1,2783) | 1:B:113:THR:HG21 | 1:B:150:PRO:HB3 | 7 | 0.3 |
| (1,2783) | 1:B:113:THR:HG22 | 1:B:150:PRO:HB3 | 7 | 0.3 |
| (1,2783) | 1:B:113:THR:HG23 | 1:B:150:PRO:HB3 | 7 | 0.3 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD11 | 7 | 0.3 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD12 | 7 | 0.3 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD13 | 7 | 0.3 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 5 | 0.3 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 3 | 0.3 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE1 | 6 | 0.3 |
| (1,2535) | 1:B:99:LEU:HD21 | 1:B:142:TYR:HE2 | 6 | 0.3 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE1 | 6 | 0.3 |
| (1,2535) | 1:B:99:LEU:HD22 | 1:B:142:TYR:HE2 | 6 | 0.3 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE1 | 6 | 0.3 |
| (1,2535) | 1:B:99:LEU:HD23 | 1:B:142:TYR:HE2 | 6 | 0.3 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 9 | 0.3 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 9 | 0.3 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 9 | 0.3 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 7 | 0.3 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 7 | 0.3 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 7 | 0.3 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 8 | 0.3 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 8 | 0.3 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 8 | 0.3 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 5 | 0.3 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 5 | 0.3 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 5 | 0.3 |
| (1,2312) | 1:B:94:ARG:HA | 1:B:168:PRO:HD2 | 2 | 0.3 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB1 | 2 | 0.3 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB2 | 2 | 0.3 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB3 | 2 | 0.3 |
| (1,2284) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB2 | 1 | 0.3 |
| (1,2284) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB2 | 1 | 0.3 |
| (1,1915) | 1:A:162:THR:H | 1:A:102:ASN:HB2 | 10 | 0.3 |
| (1,19) | 1:A:93:ASP:HB2 | 1:A:94:ARG:HG2 | 2 | 0.3 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 2 | 0.3 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 4 | 0.3 |
| (1,1847) | 1:A:155:SER:H | 1:A:154:SER:HB2 | 7 | 0.3 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 8 | 0.3 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 8 | 0.3 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 8 | 0.3 |
| (1,1654) | 1:A:134:ILE:H | 1:A:127:ARG:HB2 | 2 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1598) | 1:A:128:GLN:H | 1:A:127:ARG:HG2 | 7 | 0.3 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 9 | 0.3 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 6 | 0.3 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 8 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 2 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 2 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 2 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 2 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 2 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 2 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 9 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 9 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 9 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 9 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 9 | 0.3 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 9 | 0.3 |
| (1,1411) | 1:A:108:GLU:H | 1:A:105:ALA:HA | 6 | 0.3 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 2 | 0.3 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 3 | 0.3 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 2 | 0.3 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 2 | 0.3 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 2 | 0.3 |
| (1,1219) | 1:A:162:THR:HA | 1:A:162:THR:HG21 | 2 | 0.3 |
| (1,1219) | 1:A:162:THR:HA | 1:A:162:THR:HG22 | 2 | 0.3 |
| (1,1219) | 1:A:162:THR:HA | 1:A:162:THR:HG23 | 2 | 0.3 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 10 | 0.3 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 1 | 0.3 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 3 | 0.3 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 3 | 0.3 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 3 | 0.3 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 1 | 0.3 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 10 | 0.3 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 8 | 0.3 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 8 | 0.3 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 8 | 0.3 |
| (1,1012) | 1:A:148:VAL:HG11 | 1:A:169:MET:HB2 | 2 | 0.3 |
| (1,1012) | 1:A:148:VAL:HG12 | 1:A:169:MET:HB2 | 2 | 0.3 |
| (1,1012) | 1:A:148:VAL:HG13 | 1:A:169:MET:HB2 | 2 | 0.3 |
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 6 | 0.29 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 6 | 0.29 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 6 | 0.29 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 6 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG11 | 8 | 0.29 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG12 | 8 | 0.29 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG13 | 8 | 0.29 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG11 | 8 | 0.29 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG12 | 8 | 0.29 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG13 | 8 | 0.29 |
| (1,847) | 1:A:141:LYS:HA | 1:A:141:LYS:HE3 | 6 | 0.29 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 2 | 0.29 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 2 | 0.29 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 2 | 0.29 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 8 | 0.29 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 8 | 0.29 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 8 | 0.29 |
| (1,808) | 1:A:135:SER:HA | 1:A:135:SER:HB2 | 5 | 0.29 |
| (1,715) | 1:A:126:GLU:HB2 | 1:A:135:SER:HB3 | 6 | 0.29 |
| (1,715) | 1:A:126:GLU:HB3 | 1:A:135:SER:HB3 | 6 | 0.29 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 7 | 0.29 |
| (1,688) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB3 | 2 | 0.29 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 10 | 0.29 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 10 | 0.29 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 10 | 0.29 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 10 | 0.29 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 10 | 0.29 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 10 | 0.29 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 10 | 0.29 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 10 | 0.29 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 10 | 0.29 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 8 | 0.29 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 8 | 0.29 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 8 | 0.29 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG2 | 7 | 0.29 |
| (1,4297) | 1:B:174:THR:H | 1:B:171:LYS:HG3 | 7 | 0.29 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 6 | 0.29 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 6 | 0.29 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 6 | 0.29 |
| (1,3972) | 1:B:140:ARG:H | 1:B:120:ILE:HB | 6 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 3 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 3 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 3 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 3 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 3 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 3 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 5 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 5 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 5 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 5 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 5 | 0.29 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 5 | 0.29 |
| (1,3894) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HA | 1 | 0.29 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 6 | 0.29 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 6 | 0.29 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 2 | 0.29 |
| (1,3748) | 1:B:113:THR:H | 1:B:112:LYS:HB2 | 2 | 0.29 |
| (1,3726) | 1:B:111:VAL:H | 1:B:110:THR:HB | 7 | 0.29 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 7 | 0.29 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 5 | 0.29 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 7 | 0.29 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 7 | 0.29 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 7 | 0.29 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 5 | 0.29 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 1 | 0.29 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 7 | 0.29 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 9 | 0.29 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 9 | 0.29 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 9 | 0.29 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 9 | 0.29 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 9 | 0.29 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 9 | 0.29 |
| (1,324) | 1:A:106:PRO:HB3 | 1:A:107:ASP:HA | 9 | 0.29 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 2 | 0.29 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 2 | 0.29 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 2 | 0.29 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG21 | 4 | 0.29 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG22 | 4 | 0.29 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG23 | 4 | 0.29 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD3 | 7 | 0.29 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD2 | 7 | 0.29 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 5 | 0.29 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 5 | 0.29 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 5 | 0.29 |
| (1,3139) | 1:B:141:LYS:HG3 | 1:B:141:LYS:HE2 | 8 | 0.29 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD1 | 7 | 0.29 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD2 | 7 | 0.29 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD1 | 7 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD2 | 7 | 0.29 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD1 | 7 | 0.29 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD2 | 7 | 0.29 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 7 | 0.29 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 10 | 0.29 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 10 | 0.29 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 10 | 0.29 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG21 | 10 | 0.29 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG22 | 10 | 0.29 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG23 | 10 | 0.29 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 3 | 0.29 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 3 | 0.29 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 3 | 0.29 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 4 | 0.29 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 4 | 0.29 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 4 | 0.29 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD11 | 8 | 0.29 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD12 | 8 | 0.29 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD13 | 8 | 0.29 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 1 | 0.29 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 8 | 0.29 |
| (1,258) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HA | 2 | 0.29 |
| (1,258) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HA | 2 | 0.29 |
| (1,258) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HA | 2 | 0.29 |
| (1,258) | 1:A:99:LEU:HD21 | 1:A:120:ILE:HA | 2 | 0.29 |
| (1,258) | 1:A:99:LEU:HD22 | 1:A:120:ILE:HA | 2 | 0.29 |
| (1,258) | 1:A:99:LEU:HD23 | 1:A:120:ILE:HA | 2 | 0.29 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 10 | 0.29 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 10 | 0.29 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 10 | 0.29 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 2 | 0.29 |
| (1,2383) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HB3 | 2 | 0.29 |
| (1,2383) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HB3 | 4 | 0.29 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB1 | 10 | 0.29 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB2 | 10 | 0.29 |
| (1,2358) | 1:B:95:TRP:HE3 | 1:B:167:ALA:HB3 | 10 | 0.29 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 1 | 0.29 |
| (1,2284) | 1:B:89:ARG:HB2 | 1:B:90:HIS:HB2 | 10 | 0.29 |
| (1,2284) | 1:B:89:ARG:HB3 | 1:B:90:HIS:HB2 | 10 | 0.29 |
| (1,2150) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2150) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2150) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 6 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2150) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2150) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2150) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2018) | 1:B:97:VAL:HG21 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2018) | 1:B:97:VAL:HG22 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2018) | 1:B:97:VAL:HG23 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2018) | 1:B:97:VAL:HG11 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2018) | 1:B:97:VAL:HG12 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,2018) | 1:B:97:VAL:HG13 | 1:A:131:HIS:HB3 | 6 | 0.29 |
| (1,1998) | 1:A:169:MET:H | 1:A:169:MET:HB2 | 8 | 0.29 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 10 | 0.29 |
| (1,1847) | 1:A:155:SER:H | 1:A:154:SER:HB2 | 4 | 0.29 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 7 | 0.29 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 7 | 0.29 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 7 | 0.29 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 7 | 0.29 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 7 | 0.29 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 7 | 0.29 |
| (1,1650) | 1:A:132:GLY:H | 1:A:133:TYR:HD1 | 1 | 0.29 |
| (1,1650) | 1:A:132:GLY:H | 1:A:133:TYR:HD2 | 1 | 0.29 |
| (1,1621) | 1:A:129:ASP:H | 1:A:129:ASP:HB2 | 1 | 0.29 |
| (1,1500) | 1:A:117:VAL:H | 1:A:115:ASP:HB2 | 10 | 0.29 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 7 | 0.29 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD11 | 4 | 0.29 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD12 | 4 | 0.29 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD13 | 4 | 0.29 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD21 | 4 | 0.29 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD22 | 4 | 0.29 |
| (1,1432) | 1:A:109:LEU:H | 1:A:157:LEU:HD23 | 4 | 0.29 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD11 | 10 | 0.29 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD12 | 10 | 0.29 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD13 | 10 | 0.29 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD21 | 1 | 0.29 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD22 | 1 | 0.29 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD23 | 1 | 0.29 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 7 | 0.29 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 7 | 0.29 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 7 | 0.29 |
| (1,1276) | 1:A:168:PRO:HA | 1:A:169:MET:HG2 | 9 | 0.29 |
| (1,1258) | 1:A:166:GLU:HG2 | 1:A:167:ALA:HA | 8 | 0.29 |
| (1,1258) | 1:A:166:GLU:HG3 | 1:A:167:ALA:HA | 8 | 0.29 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 1 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 5 | 0.29 |
| (1,1149) | 1:A:157:LEU:HA | 1:A:163:LEU:HB3 | 1 | 0.29 |
| (1,1149) | 1:A:157:LEU:HA | 1:A:163:LEU:HB3 | 6 | 0.29 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 9 | 0.29 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 3 | 0.29 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 7 | 0.29 |
| (1,1065) | 1:A:152:GLN:HB2 | 1:A:169:MET:HA | 7 | 0.29 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 2 | 0.29 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 6 | 0.29 |
| (1,102) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HB3 | 1 | 0.29 |
| (1,1012) | 1:A:148:VAL:HG11 | 1:A:169:MET:HB2 | 6 | 0.29 |
| (1,1012) | 1:A:148:VAL:HG12 | 1:A:169:MET:HB2 | 6 | 0.29 |
| (1,1012) | 1:A:148:VAL:HG13 | 1:A:169:MET:HB2 | 6 | 0.29 |
| (1,990) | 1:A:148:VAL:HA | 1:A:169:MET:HB2 | 2 | 0.28 |
| (1,958) | 1:A:145:PRO:HG3 | 1:A:146:PRO:HD2 | 6 | 0.28 |
| (1,9) | 1:A:90:HIS:HB3 | 1:A:91:THR:HA | 7 | 0.28 |
| (1,831) | 1:A:139:THR:HB | 1:A:141:LYS:HE2 | 8 | 0.28 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 5 | 0.28 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 5 | 0.28 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 5 | 0.28 |
| (1,718) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HB3 | 6 | 0.28 |
| (1,687) | 1:A:123:LYS:HB2 | 1:A:137:CYS:HB2 | 10 | 0.28 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG21 | 3 | 0.28 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG22 | 3 | 0.28 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG23 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 3 | 0.28 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 7 | 0.28 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 7 | 0.28 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 7 | 0.28 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 7 | 0.28 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 7 | 0.28 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 7 | 0.28 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 7 | 0.28 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 7 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 7 | 0.28 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD2 | 3 | 0.28 |
| (1,4288) | 1:B:171:LYS:H | 1:B:170:PRO:HD3 | 3 | 0.28 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG2 | 9 | 0.28 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG3 | 9 | 0.28 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE1 | 1 | 0.28 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE2 | 1 | 0.28 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE1 | 2 | 0.28 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE2 | 2 | 0.28 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 3 | 0.28 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 7 | 0.28 |
| (1,3748) | 1:B:113:THR:H | 1:B:112:LYS:HB2 | 3 | 0.28 |
| (1,3748) | 1:B:113:THR:H | 1:B:112:LYS:HB2 | 9 | 0.28 |
| (1,3726) | 1:B:111:VAL:H | 1:B:110:THR:HB | 1 | 0.28 |
| (1,3726) | 1:B:111:VAL:H | 1:B:110:THR:HB | 6 | 0.28 |
| (1,3654) | 1:B:102:ASN:HD21 | 1:B:161:GLY:HA2 | 6 | 0.28 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 3 | 0.28 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 3 | 0.28 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 3 | 0.28 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 3 | 0.28 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 3 | 0.28 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 3 | 0.28 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 4 | 0.28 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 4 | 0.28 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 4 | 0.28 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD2 | 9 | 0.28 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD2 | 9 | 0.28 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD3 | 9 | 0.28 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD3 | 9 | 0.28 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD3 | 10 | 0.28 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD2 | 10 | 0.28 |
| (1,346) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HG3 | 8 | 0.28 |
| (1,346) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HG2 | 8 | 0.28 |
| (1,3454) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB3 | 9 | 0.28 |
| (1,3454) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB3 | 9 | 0.28 |
| (1,3454) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB3 | 9 | 0.28 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 1 | 0.28 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 1 | 0.28 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 1 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG11 | 1:B:155:SER:HB3 | 5 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG12 | 1:B:155:SER:HB3 | 5 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG13 | 1:B:155:SER:HB3 | 5 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3366) | 1:B:153:VAL:HG21 | 1:B:155:SER:HB3 | 5 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG22 | 1:B:155:SER:HB3 | 5 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG23 | 1:B:155:SER:HB3 | 5 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG11 | 1:B:155:SER:HB3 | 6 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG12 | 1:B:155:SER:HB3 | 6 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG13 | 1:B:155:SER:HB3 | 6 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG21 | 1:B:155:SER:HB3 | 6 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG22 | 1:B:155:SER:HB3 | 6 | 0.28 |
| (1,3366) | 1:B:153:VAL:HG23 | 1:B:155:SER:HB3 | 6 | 0.28 |
| (1,336) | 1:A:108:GLU:HA | 1:A:108:GLU:HG2 | 4 | 0.28 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 2 | 0.28 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 3 | 0.28 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 8 | 0.28 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 1 | 0.28 |
| (1,3211) | 1:B:144:LEU:HD11 | 1:B:148:VAL:HA | 7 | 0.28 |
| (1,3211) | 1:B:144:LEU:HD12 | 1:B:148:VAL:HA | 7 | 0.28 |
| (1,3211) | 1:B:144:LEU:HD13 | 1:B:148:VAL:HA | 7 | 0.28 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG21 | 5 | 0.28 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG22 | 5 | 0.28 |
| (1,3201) | 1:B:144:LEU:HB3 | 1:B:148:VAL:HG23 | 5 | 0.28 |
| (1,3138) | 1:B:141:LYS:HG2 | 1:B:143:THR:HA | 3 | 0.28 |
| (1,3137) | 1:B:141:LYS:HG2 | 1:B:142:TYR:HB3 | 3 | 0.28 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD1 | 9 | 0.28 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD2 | 9 | 0.28 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD1 | 9 | 0.28 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD2 | 9 | 0.28 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD1 | 9 | 0.28 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD2 | 9 | 0.28 |
| (1,3053) | 1:B:130:GLU:HA | 1:B:130:GLU:HG2 | 4 | 0.28 |
| (1,3003) | 1:B:126:GLU:HG2 | 1:B:135:SER:HA | 1 | 0.28 |
| (1,3003) | 1:B:126:GLU:HG2 | 1:B:135:SER:HA | 5 | 0.28 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 9 | 0.28 |
| (1,2935) | 1:B:120:ILE:HD11 | 1:B:140:ARG:HD2 | 2 | 0.28 |
| (1,2935) | 1:B:120:ILE:HD12 | 1:B:140:ARG:HD2 | 2 | 0.28 |
| (1,2935) | 1:B:120:ILE:HD13 | 1:B:140:ARG:HD2 | 2 | 0.28 |
| (1,2928) | 1:B:120:ILE:HG21 | 1:B:122:GLY:HA3 | 6 | 0.28 |
| (1,2928) | 1:B:120:ILE:HG22 | 1:B:122:GLY:HA3 | 6 | 0.28 |
| (1,2928) | 1:B:120:ILE:HG23 | 1:B:122:GLY:HA3 | 6 | 0.28 |
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 4 | 0.28 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 1 | 0.28 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 1 | 0.28 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 1 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 7 | 0.28 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 7 | 0.28 |
| (1,2738) | 1:B:112:LYS:HB2 | 1:B:120:ILE:HA | 1 | 0.28 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 5 | 0.28 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 5 | 0.28 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 5 | 0.28 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 2 | 0.28 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 2 | 0.28 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 2 | 0.28 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG21 | 6 | 0.28 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG22 | 6 | 0.28 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG23 | 6 | 0.28 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 5 | 0.28 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 4 | 0.28 |
| (1,2539) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HA | 3 | 0.28 |
| (1,2539) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HA | 3 | 0.28 |
| (1,2539) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HA | 3 | 0.28 |
| (1,2539) | 1:B:99:LEU:HD21 | 1:B:120:ILE:HA | 3 | 0.28 |
| (1,2539) | 1:B:99:LEU:HD22 | 1:B:120:ILE:HA | 3 | 0.28 |
| (1,2539) | 1:B:99:LEU:HD23 | 1:B:120:ILE:HA | 3 | 0.28 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 2 | 0.28 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 4 | 0.28 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 4 | 0.28 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 4 | 0.28 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 6 | 0.28 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 6 | 0.28 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 6 | 0.28 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 9 | 0.28 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 9 | 0.28 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 9 | 0.28 |
| (1,232) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HG12 | 8 | 0.28 |
| (1,232) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HG12 | 8 | 0.28 |
| (1,232) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HG12 | 8 | 0.28 |
| (1,2318) | 1:B:94:ARG:HB2 | 1:B:96:ARG:HA | 2 | 0.28 |
| (1,2282) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HA | 5 | 0.28 |
| (1,2282) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HA | 5 | 0.28 |
| (1,2282) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HA | 5 | 0.28 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD2 | 5 | 0.28 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD3 | 5 | 0.28 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 8 | 0.28 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 3 | 0.28 |
| (1,1847) | 1:A:155:SER:H | 1:A:154:SER:HB2 | 10 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 9 | 0.28 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 6 | 0.28 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 6 | 0.28 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 6 | 0.28 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 1 | 0.28 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 1 | 0.28 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 1 | 0.28 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 1 | 0.28 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 1 | 0.28 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 1 | 0.28 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 10 | 0.28 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 8 | 0.28 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 8 | 0.28 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 6 | 0.28 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 6 | 0.28 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 6 | 0.28 |
| (1,1323) | 1:A:94:ARG:H | 1:A:93:ASP:HB3 | 6 | 0.28 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 4 | 0.28 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 7 | 0.28 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 8 | 0.28 |
| (1,1102) | 1:A:155:SER:HA | 1:A:155:SER:HB3 | 7 | 0.28 |
| (1,1097) | 1:A:154:SER:HB3 | 1:A:155:SER:HA | 5 | 0.28 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 6 | 0.28 |
| (1,102) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HB3 | 7 | 0.28 |
| (1,99) | 1:A:96:ARG:HB3 | 1:A:164:THR:HB | 10 | 0.27 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG3 | 5 | 0.27 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG2 | 5 | 0.27 |
| (1,917) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA2 | 1 | 0.27 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 2 | 0.27 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 2 | 0.27 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 2 | 0.27 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 7 | 0.27 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 7 | 0.27 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 7 | 0.27 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 5 | 0.27 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 5 | 0.27 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 5 | 0.27 |
| (1,837) | 1:A:140:ARG:HA | 1:A:140:ARG:HD3 | 8 | 0.27 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 4 | 0.27 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 4 | 0.27 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 4 | 0.27 |
| (1,808) | 1:A:135:SER:HA | 1:A:135:SER:HB2 | 2 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,782) | 1:A:131:HIS:HB2 | 1:A:132:GLY:HA2 | 8 | 0.27 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 1 | 0.27 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 8 | 0.27 |
| (1,689) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HA | 8 | 0.27 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 3 | 0.27 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 3 | 0.27 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 3 | 0.27 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 5 | 0.27 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 5 | 0.27 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 5 | 0.27 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 10 | 0.27 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 10 | 0.27 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 10 | 0.27 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG21 | 5 | 0.27 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG22 | 5 | 0.27 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG23 | 5 | 0.27 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG11 | 7 | 0.27 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG12 | 7 | 0.27 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG13 | 7 | 0.27 |
| (1,51) | 1:A:95:TRP:HA | 1:A:95:TRP:HB2 | 4 | 0.27 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 8 | 0.27 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD2 | 2 | 0.27 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD3 | 2 | 0.27 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG2 | 5 | 0.27 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG3 | 5 | 0.27 |
| (1,4263) | 1:B:167:ALA:H | 1:B:166:GLU:HB3 | 6 | 0.27 |
| (1,4262) | 1:B:167:ALA:H | 1:B:166:GLU:HB2 | 5 | 0.27 |
| (1,3935) | 1:B:134:ILE:H | 1:B:127:ARG:HB2 | 7 | 0.27 |
| (1,3918) | 1:B:131:HIS:H | 1:B:130:GLU:HG2 | 10 | 0.27 |
| (1,3918) | 1:B:131:HIS:H | 1:B:130:GLU:HG3 | 10 | 0.27 |
| (1,3902) | 1:B:129:ASP:H | 1:B:129:ASP:HB2 | 8 | 0.27 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 1 | 0.27 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 1 | 0.27 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD21 | 3 | 0.27 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD22 | 3 | 0.27 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD23 | 3 | 0.27 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 10 | 0.27 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 10 | 0.27 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 10 | 0.27 |
| (1,3590) | 1:B:170:PRO:HA | 1:B:170:PRO:HD2 | 3 | 0.27 |
| (1,3590) | 1:B:170:PRO:HA | 1:B:170:PRO:HD3 | 3 | 0.27 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 6 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 9 | 0.27 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 9 | 0.27 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 9 | 0.27 |
| (1,3566) | 1:B:168:PRO:HD2 | 1:B:169:MET:HA | 2 | 0.27 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 10 | 0.27 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 9 | 0.27 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 1 | 0.27 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD21 | 7 | 0.27 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD22 | 7 | 0.27 |
| (1,3403) | 1:B:155:SER:HB3 | 1:B:157:LEU:HD23 | 7 | 0.27 |
| (1,3395) | 1:B:155:SER:HB2 | 1:B:163:LEU:HA | 5 | 0.27 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD11 | 6 | 0.27 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD12 | 6 | 0.27 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD13 | 6 | 0.27 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD21 | 6 | 0.27 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD22 | 6 | 0.27 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD23 | 6 | 0.27 |
| (1,3383) | 1:B:155:SER:HA | 1:B:155:SER:HB3 | 10 | 0.27 |
| (1,3345) | 1:B:152:GLN:HB2 | 1:B:168:PRO:HD3 | 6 | 0.27 |
| (1,3274) | 1:B:148:VAL:HA | 1:B:170:PRO:HG2 | 10 | 0.27 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 7 | 0.27 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 7 | 0.27 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 7 | 0.27 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 5 | 0.27 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 5 | 0.27 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 5 | 0.27 |
| (1,3092) | 1:B:136:ARG:HA | 1:B:136:ARG:HG2 | 4 | 0.27 |
| (1,2931) | 1:B:120:ILE:HG21 | 1:B:142:TYR:HD1 | 2 | 0.27 |
| (1,2931) | 1:B:120:ILE:HG21 | 1:B:142:TYR:HD2 | 2 | 0.27 |
| (1,2931) | 1:B:120:ILE:HG22 | 1:B:142:TYR:HD1 | 2 | 0.27 |
| (1,2931) | 1:B:120:ILE:HG22 | 1:B:142:TYR:HD2 | 2 | 0.27 |
| (1,2931) | 1:B:120:ILE:HG23 | 1:B:142:TYR:HD1 | 2 | 0.27 |
| (1,2931) | 1:B:120:ILE:HG23 | 1:B:142:TYR:HD2 | 2 | 0.27 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 1 | 0.27 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 1 | 0.27 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 1 | 0.27 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 9 | 0.27 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 9 | 0.27 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 9 | 0.27 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG21 | 7 | 0.27 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG22 | 7 | 0.27 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG23 | 7 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG21 | 9 | 0.27 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG22 | 9 | 0.27 |
| (1,2919) | 1:B:120:ILE:HG12 | 1:B:120:ILE:HG23 | 9 | 0.27 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD11 | 4 | 0.27 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD12 | 4 | 0.27 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD13 | 4 | 0.27 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 1 | 0.27 |
| (1,2613) | 1:B:107:ASP:HA | 1:B:108:GLU:HG3 | 6 | 0.27 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 9 | 0.27 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 9 | 0.27 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 9 | 0.27 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 5 | 0.27 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 5 | 0.27 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 5 | 0.27 |
| (1,2332) | 1:B:95:TRP:HA | 1:B:95:TRP:HB2 | 8 | 0.27 |
| (1,2313) | 1:B:94:ARG:HA | 1:B:168:PRO:HD3 | 1 | 0.27 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG21 | 8 | 0.27 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG22 | 8 | 0.27 |
| (1,2287) | 1:B:90:HIS:HA | 1:B:91:THR:HG23 | 8 | 0.27 |
| (1,2281) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 6 | 0.27 |
| (1,2213) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 6 | 0.27 |
| (1,2192) | 1:B:134:ILE:HA | 1:A:140:ARG:HG3 | 4 | 0.27 |
| (1,2148) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 6 | 0.27 |
| (1,2081) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 6 | 0.27 |
| (1,2060) | 1:B:134:ILE:HA | 1:A:140:ARG:HG3 | 4 | 0.27 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 9 | 0.27 |
| (1,1626) | 1:A:129:ASP:H | 1:A:132:GLY:HA3 | 9 | 0.27 |
| (1,1584) | 1:A:125:GLU:H | 1:A:126:GLU:H | 2 | 0.27 |
| (1,1580) | 1:A:125:GLU:H | 1:A:108:GLU:HG2 | 7 | 0.27 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 3 | 0.27 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 4 | 0.27 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 1 | 0.27 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 1 | 0.27 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 5 | 0.27 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD11 | 8 | 0.27 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD12 | 8 | 0.27 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD13 | 8 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 4 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 4 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 4 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 4 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 4 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 4 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 9 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 9 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 9 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 9 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 9 | 0.27 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 9 | 0.27 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 7 | 0.27 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 7 | 0.27 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 7 | 0.27 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 6 | 0.27 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 9 | 0.27 |
| (1,1168) | 1:A:157:LEU:HD11 | 1:A:161:GLY:HA3 | 3 | 0.27 |
| (1,1168) | 1:A:157:LEU:HD12 | 1:A:161:GLY:HA3 | 3 | 0.27 |
| (1,1168) | 1:A:157:LEU:HD13 | 1:A:161:GLY:HA3 | 3 | 0.27 |
| (1,1097) | 1:A:154:SER:HB3 | 1:A:155:SER:HA | 6 | 0.27 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 3 | 0.27 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 3 | 0.27 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 10 | 0.27 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG11 | 6 | 0.26 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG12 | 6 | 0.26 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG13 | 6 | 0.26 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG3 | 7 | 0.26 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG2 | 7 | 0.26 |
| (1,93) | 1:A:96:ARG:HB2 | 1:A:96:ARG:HD3 | 10 | 0.26 |
| (1,93) | 1:A:96:ARG:HB2 | 1:A:96:ARG:HD2 | 10 | 0.26 |
| (1,9) | 1:A:90:HIS:HB3 | 1:A:91:THR:HA | 5 | 0.26 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 10 | 0.26 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 10 | 0.26 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 10 | 0.26 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 5 | 0.26 |
| (1,839) | 1:A:140:ARG:HB2 | 1:A:140:ARG:HD2 | 1 | 0.26 |
| (1,839) | 1:A:140:ARG:HB3 | 1:A:140:ARG:HD2 | 1 | 0.26 |
| (1,831) | 1:A:139:THR:HB | 1:A:141:LYS:HE2 | 6 | 0.26 |
| (1,808) | 1:A:135:SER:HA | 1:A:135:SER:HB2 | 3 | 0.26 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 8 | 0.26 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 8 | 0.26 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 8 | 0.26 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 10 | 0.26 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG11 | 5 | 0.26 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG12 | 5 | 0.26 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG13 | 5 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 10 | 0.26 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 10 | 0.26 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 10 | 0.26 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 10 | 0.26 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 10 | 0.26 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 10 | 0.26 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 4 | 0.26 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 4 | 0.26 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 4 | 0.26 |
| (1,51) | 1:A:95:TRP:HA | 1:A:95:TRP:HB2 | 7 | 0.26 |
| (1,434) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG12 | 9 | 0.26 |
| (1,434) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG12 | 9 | 0.26 |
| (1,434) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG12 | 9 | 0.26 |
| (1,434) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG12 | 9 | 0.26 |
| (1,434) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG12 | 9 | 0.26 |
| (1,434) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG12 | 9 | 0.26 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 1 | 0.26 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 7 | 0.26 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 7 | 0.26 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 7 | 0.26 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 7 | 0.26 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 7 | 0.26 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 7 | 0.26 |
| (1,3915) | 1:B:131:HIS:H | 1:B:129:ASP:HB3 | 9 | 0.26 |
| (1,3907) | 1:B:129:ASP:H | 1:B:132:GLY:HA3 | 3 | 0.26 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 10 | 0.26 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 10 | 0.26 |
| (1,3862) | 1:B:125:GLU:H | 1:B:108:GLU:HG3 | 5 | 0.26 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 9 | 0.26 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 10 | 0.26 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 3 | 0.26 |
| (1,3672) | 1:B:105:ALA:H | 1:B:108:GLU:HB3 | 2 | 0.26 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD21 | 8 | 0.26 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD22 | 8 | 0.26 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD23 | 8 | 0.26 |
| (1,3614) | 1:B:95:TRP:H | 1:B:166:GLU:HG2 | 9 | 0.26 |
| (1,3614) | 1:B:95:TRP:H | 1:B:166:GLU:HG3 | 9 | 0.26 |
| (1,3602) | 1:B:94:ARG:H | 1:B:93:ASP:HA | 9 | 0.26 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG21 | 1 | 0.26 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG22 | 1 | 0.26 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG23 | 1 | 0.26 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 2 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3539) | 1:B:166:GLU:HG2 | 1:B:167:ALA:HA | 9 | 0.26 |
| (1,3539) | 1:B:166:GLU:HG3 | 1:B:167:ALA:HA | 9 | 0.26 |
| (1,3409) | 1:B:155:SER:HB3 | 1:B:157:LEU:HB3 | 4 | 0.26 |
| (1,3409) | 1:B:155:SER:HB2 | 1:B:157:LEU:HB3 | 4 | 0.26 |
| (1,337) | 1:A:108:GLU:HA | 1:A:108:GLU:HG3 | 6 | 0.26 |
| (1,3346) | 1:B:152:GLN:HB2 | 1:B:169:MET:HA | 5 | 0.26 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 9 | 0.26 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 9 | 0.26 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 9 | 0.26 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 10 | 0.26 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 10 | 0.26 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 10 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG11 | 1:B:170:PRO:HG3 | 1 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG12 | 1:B:170:PRO:HG3 | 1 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG13 | 1:B:170:PRO:HG3 | 1 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG11 | 1:B:170:PRO:HG3 | 3 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG12 | 1:B:170:PRO:HG3 | 3 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG13 | 1:B:170:PRO:HG3 | 3 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG11 | 1:B:170:PRO:HG3 | 9 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG12 | 1:B:170:PRO:HG3 | 9 | 0.26 |
| (1,3295) | 1:B:148:VAL:HG13 | 1:B:170:PRO:HG3 | 9 | 0.26 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 3 | 0.26 |
| (1,3096) | 1:B:136:ARG:HG3 | 1:B:138:PHE:HA | 8 | 0.26 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 3 | 0.26 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 5 | 0.26 |
| (1,3054) | 1:B:130:GLU:HA | 1:B:130:GLU:HG3 | 3 | 0.26 |
| (1,3003) | 1:B:126:GLU:HG2 | 1:B:135:SER:HA | 3 | 0.26 |
| (1,2930) | 1:B:120:ILE:HG21 | 1:B:140:ARG:HA | 3 | 0.26 |
| (1,2930) | 1:B:120:ILE:HG22 | 1:B:140:ARG:HA | 3 | 0.26 |
| (1,2930) | 1:B:120:ILE:HG23 | 1:B:140:ARG:HA | 3 | 0.26 |
| (1,2929) | 1:B:120:ILE:HG21 | 1:B:139:THR:HA | 1 | 0.26 |
| (1,2929) | 1:B:120:ILE:HG22 | 1:B:139:THR:HA | 1 | 0.26 |
| (1,2929) | 1:B:120:ILE:HG23 | 1:B:139:THR:HA | 1 | 0.26 |
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 9 | 0.26 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 4 | 0.26 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 4 | 0.26 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 4 | 0.26 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD11 | 4 | 0.26 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD12 | 4 | 0.26 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD13 | 4 | 0.26 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD11 | 7 | 0.26 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD12 | 7 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD13 | 7 | 0.26 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 7 | 0.26 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 7 | 0.26 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 7 | 0.26 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 4 | 0.26 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 6 | 0.26 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 9 | 0.26 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 9 | 0.26 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 9 | 0.26 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD21 | 8 | 0.26 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD22 | 8 | 0.26 |
| (1,2616) | 1:B:107:ASP:HA | 1:B:157:LEU:HD23 | 8 | 0.26 |
| (1,2592) | 1:B:106:PRO:HA | 1:B:109:LEU:HB2 | 10 | 0.26 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 1 | 0.26 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 4 | 0.26 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 4 | 0.26 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 4 | 0.26 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 2 | 0.26 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 2 | 0.26 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 2 | 0.26 |
| (1,2283) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HB3 | 3 | 0.26 |
| (1,2283) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HB3 | 3 | 0.26 |
| (1,2283) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HB3 | 3 | 0.26 |
| (1,2169) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 5 | 0.26 |
| (1,2152) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2152) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2152) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2152) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2152) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2152) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2037) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 5 | 0.26 |
| (1,2020) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2020) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2020) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2020) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2020) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,2020) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 7 | 0.26 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD11 | 8 | 0.26 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD12 | 8 | 0.26 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD13 | 8 | 0.26 |
| (1,1915) | 1:A:162:THR:H | 1:A:102:ASN:HB2 | 8 | 0.26 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG21 | 5 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG22 | 5 | 0.26 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG23 | 5 | 0.26 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 5 | 0.26 |
| (1,18) | 1:A:93:ASP:HB2 | 1:A:94:ARG:HA | 3 | 0.26 |
| (1,1626) | 1:A:129:ASP:H | 1:A:132:GLY:HA3 | 7 | 0.26 |
| (1,1598) | 1:A:128:GLN:H | 1:A:127:ARG:HG2 | 3 | 0.26 |
| (1,1525) | 1:A:119:GLU:H | 1:A:114:LYS:HB3 | 3 | 0.26 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 7 | 0.26 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 2 | 0.26 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 3 | 0.26 |
| (1,1399) | 1:A:107:ASP:H | 1:A:106:PRO:HB2 | 10 | 0.26 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 9 | 0.26 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 9 | 0.26 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 9 | 0.26 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 2 | 0.26 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 5 | 0.26 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 4 | 0.26 |
| (1,1179) | 1:A:157:LEU:HD21 | 1:A:163:LEU:HB3 | 9 | 0.26 |
| (1,1179) | 1:A:157:LEU:HD22 | 1:A:163:LEU:HB3 | 9 | 0.26 |
| (1,1179) | 1:A:157:LEU:HD23 | 1:A:163:LEU:HB3 | 9 | 0.26 |
| (1,1179) | 1:A:157:LEU:HD21 | 1:A:163:LEU:HB3 | 10 | 0.26 |
| (1,1179) | 1:A:157:LEU:HD22 | 1:A:163:LEU:HB3 | 10 | 0.26 |
| (1,1179) | 1:A:157:LEU:HD23 | 1:A:163:LEU:HB3 | 10 | 0.26 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 5 | 0.26 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 5 | 0.26 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 5 | 0.26 |
| (1,1168) | 1:A:157:LEU:HD11 | 1:A:161:GLY:HA3 | 1 | 0.26 |
| (1,1168) | 1:A:157:LEU:HD12 | 1:A:161:GLY:HA3 | 1 | 0.26 |
| (1,1168) | 1:A:157:LEU:HD13 | 1:A:161:GLY:HA3 | 1 | 0.26 |
| (1,1168) | 1:A:157:LEU:HD11 | 1:A:161:GLY:HA3 | 10 | 0.26 |
| (1,1168) | 1:A:157:LEU:HD12 | 1:A:161:GLY:HA3 | 10 | 0.26 |
| (1,1168) | 1:A:157:LEU:HD13 | 1:A:161:GLY:HA3 | 10 | 0.26 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 1 | 0.26 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 4 | 0.26 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 6 | 0.26 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 9 | 0.26 |
| (1,862) | 1:A:141:LYS:HG3 | 1:A:142:TYR:HB3 | 1 | 0.25 |
| (1,827) | 1:A:139:THR:HA | 1:A:140:ARG:HG2 | 1 | 0.25 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD1 | 7 | 0.25 |
| (1,797) | 1:A:134:ILE:HG21 | 1:A:133:TYR:HD2 | 7 | 0.25 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD1 | 7 | 0.25 |
| (1,797) | 1:A:134:ILE:HG22 | 1:A:133:TYR:HD2 | 7 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD1 | 7 | 0.25 |
| (1,797) | 1:A:134:ILE:HG23 | 1:A:133:TYR:HD2 | 7 | 0.25 |
| (1,749) | 1:A:128:GLN:HA | 1:A:133:TYR:HE1 | 5 | 0.25 |
| (1,749) | 1:A:128:GLN:HA | 1:A:133:TYR:HE2 | 5 | 0.25 |
| (1,716) | 1:A:126:GLU:HG2 | 1:A:127:ARG:HG2 | 2 | 0.25 |
| (1,701) | 1:A:125:GLU:HA | 1:A:126:GLU:HG2 | 9 | 0.25 |
| (1,699) | 1:A:125:GLU:HA | 1:A:125:GLU:HG2 | 6 | 0.25 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 9 | 0.25 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 9 | 0.25 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 5 | 0.25 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 5 | 0.25 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 5 | 0.25 |
| (1,649) | 1:A:120:ILE:HG21 | 1:A:140:ARG:HA | 7 | 0.25 |
| (1,649) | 1:A:120:ILE:HG22 | 1:A:140:ARG:HA | 7 | 0.25 |
| (1,649) | 1:A:120:ILE:HG23 | 1:A:140:ARG:HA | 7 | 0.25 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 1 | 0.25 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 1 | 0.25 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 1 | 0.25 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 5 | 0.25 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 5 | 0.25 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 5 | 0.25 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 5 | 0.25 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 5 | 0.25 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 5 | 0.25 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 5 | 0.25 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 5 | 0.25 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 5 | 0.25 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 2 | 0.25 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 2 | 0.25 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 2 | 0.25 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 10 | 0.25 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 10 | 0.25 |
| (1,459) | 1:A:112:LYS:HB3 | 1:A:112:LYS:HE3 | 1 | 0.25 |
| (1,459) | 1:A:112:LYS:HB3 | 1:A:112:LYS:HE2 | 1 | 0.25 |
| (1,4281) | 1:B:169:MET:H | 1:B:169:MET:HG3 | 8 | 0.25 |
| (1,4279) | 1:B:169:MET:H | 1:B:169:MET:HB2 | 9 | 0.25 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG2 | 9 | 0.25 |
| (1,4180) | 1:B:160:GLU:H | 1:B:160:GLU:HG3 | 9 | 0.25 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 10 | 0.25 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 1 | 0.25 |
| (1,4048) | 1:B:149:ASP:H | 1:B:170:PRO:HG3 | 10 | 0.25 |
| (1,3936) | 1:B:134:ILE:H | 1:B:127:ARG:HG2 | 8 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3908) | 1:B:129:ASP:H | 1:B:132:GLY:H | 4 | 0.25 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 3 | 0.25 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 3 | 0.25 |
| (1,3896) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HB3 | 1 | 0.25 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD1 | 6 | 0.25 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD2 | 6 | 0.25 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 3 | 0.25 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 3 | 0.25 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 7 | 0.25 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 7 | 0.25 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 7 | 0.25 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 8 | 0.25 |
| (1,3748) | 1:B:113:THR:H | 1:B:112:LYS:HB2 | 7 | 0.25 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB2 | 4 | 0.25 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB3 | 4 | 0.25 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD11 | 10 | 0.25 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD12 | 10 | 0.25 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD13 | 10 | 0.25 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD21 | 7 | 0.25 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD22 | 7 | 0.25 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD23 | 7 | 0.25 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD11 | 7 | 0.25 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD12 | 7 | 0.25 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD13 | 7 | 0.25 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD11 | 1 | 0.25 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD12 | 1 | 0.25 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD13 | 1 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 9 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 9 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 9 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 9 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 9 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 9 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 10 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 10 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 10 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 10 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 10 | 0.25 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 10 | 0.25 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 6 | 0.25 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 6 | 0.25 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 6 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3605) | 1:B:94:ARG:H | 1:B:94:ARG:HG2 | 4 | 0.25 |
| (1,3605) | 1:B:94:ARG:H | 1:B:94:ARG:HG3 | 4 | 0.25 |
| (1,3604) | 1:B:94:ARG:H | 1:B:93:ASP:HB3 | 2 | 0.25 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 6 | 0.25 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 6 | 0.25 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 6 | 0.25 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 4 | 0.25 |
| (1,3436) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HA | 8 | 0.25 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 1 | 0.25 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 6 | 0.25 |
| (1,3302) | 1:B:148:VAL:HG21 | 1:B:169:MET:HB3 | 3 | 0.25 |
| (1,3302) | 1:B:148:VAL:HG22 | 1:B:169:MET:HB3 | 3 | 0.25 |
| (1,3302) | 1:B:148:VAL:HG23 | 1:B:169:MET:HB3 | 3 | 0.25 |
| (1,3302) | 1:B:148:VAL:HG21 | 1:B:169:MET:HB3 | 10 | 0.25 |
| (1,3302) | 1:B:148:VAL:HG22 | 1:B:169:MET:HB3 | 10 | 0.25 |
| (1,3302) | 1:B:148:VAL:HG23 | 1:B:169:MET:HB3 | 10 | 0.25 |
| (1,3295) | 1:B:148:VAL:HG11 | 1:B:170:PRO:HG3 | 2 | 0.25 |
| (1,3295) | 1:B:148:VAL:HG12 | 1:B:170:PRO:HG3 | 2 | 0.25 |
| (1,3295) | 1:B:148:VAL:HG13 | 1:B:170:PRO:HG3 | 2 | 0.25 |
| (1,3295) | 1:B:148:VAL:HG11 | 1:B:170:PRO:HG3 | 10 | 0.25 |
| (1,3295) | 1:B:148:VAL:HG12 | 1:B:170:PRO:HG3 | 10 | 0.25 |
| (1,3295) | 1:B:148:VAL:HG13 | 1:B:170:PRO:HG3 | 10 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 1 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 1 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 1 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 1 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 1 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 1 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 3 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 3 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 3 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 3 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 3 | 0.25 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 3 | 0.25 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 10 | 0.25 |
| (1,3164) | 1:B:142:TYR:HD1 | 1:B:165:VAL:HG21 | 2 | 0.25 |
| (1,3164) | 1:B:142:TYR:HD1 | 1:B:165:VAL:HG22 | 2 | 0.25 |
| (1,3164) | 1:B:142:TYR:HD1 | 1:B:165:VAL:HG23 | 2 | 0.25 |
| (1,3164) | 1:B:142:TYR:HD2 | 1:B:165:VAL:HG21 | 2 | 0.25 |
| (1,3164) | 1:B:142:TYR:HD2 | 1:B:165:VAL:HG22 | 2 | 0.25 |
| (1,3164) | 1:B:142:TYR:HD2 | 1:B:165:VAL:HG23 | 2 | 0.25 |
| (1,3120) | 1:B:140:ARG:HB2 | 1:B:140:ARG:HD2 | 8 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3120) | 1:B:140:ARG:HB3 | 1:B:140:ARG:HD2 | 8 | 0.25 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD1 | 2 | 0.25 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD2 | 2 | 0.25 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD1 | 2 | 0.25 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD2 | 2 | 0.25 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD1 | 2 | 0.25 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD2 | 2 | 0.25 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 1 | 0.25 |
| (1,3058) | 1:B:131:HIS:HA | 1:B:131:HIS:HB3 | 4 | 0.25 |
| (1,2968) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB2 | 4 | 0.25 |
| (1,2965) | 1:B:123:LYS:HA | 1:B:135:SER:HB3 | 10 | 0.25 |
| (1,2935) | 1:B:120:ILE:HD11 | 1:B:140:ARG:HD2 | 5 | 0.25 |
| (1,2935) | 1:B:120:ILE:HD12 | 1:B:140:ARG:HD2 | 5 | 0.25 |
| (1,2935) | 1:B:120:ILE:HD13 | 1:B:140:ARG:HD2 | 5 | 0.25 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 7 | 0.25 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 7 | 0.25 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 7 | 0.25 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 1 | 0.25 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 1 | 0.25 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 1 | 0.25 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 1 | 0.25 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 1 | 0.25 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 1 | 0.25 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 7 | 0.25 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 7 | 0.25 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 7 | 0.25 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 7 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 10 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 10 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 10 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 10 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 10 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 10 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 10 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 10 | 0.25 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 10 | 0.25 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 1 | 0.25 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 1 | 0.25 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 1 | 0.25 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD3 | 10 | 0.25 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD2 | 10 | 0.25 |
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 2 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2605) | 1:B:106:PRO:HB3 | 1:B:107:ASP:HA | 10 | 0.25 |
| (1,2568) | 1:B:105:ALA:HA | 1:B:108:GLU:HB3 | 5 | 0.25 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 5 | 0.25 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 8 | 0.25 |
| (1,2529) | 1:B:99:LEU:HD21 | 1:B:140:ARG:HD2 | 8 | 0.25 |
| (1,2529) | 1:B:99:LEU:HD22 | 1:B:140:ARG:HD2 | 8 | 0.25 |
| (1,2529) | 1:B:99:LEU:HD23 | 1:B:140:ARG:HD2 | 8 | 0.25 |
| (1,2383) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HB3 | 1 | 0.25 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 4 | 0.25 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 1 | 0.25 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 1 | 0.25 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 1 | 0.25 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 10 | 0.25 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 10 | 0.25 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 10 | 0.25 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 7 | 0.25 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 4 | 0.25 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 4 | 0.25 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 4 | 0.25 |
| (1,2322) | 1:B:94:ARG:HB3 | 1:B:167:ALA:HA | 2 | 0.25 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD3 | 3 | 0.25 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD2 | 3 | 0.25 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 1 | 0.25 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 1 | 0.25 |
| (1,2015) | 1:A:173:ALA:H | 1:A:172:LEU:HG | 9 | 0.25 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB2 | 9 | 0.25 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB3 | 9 | 0.25 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 5 | 0.25 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 5 | 0.25 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 5 | 0.25 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 5 | 0.25 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 5 | 0.25 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 5 | 0.25 |
| (1,19) | 1:A:93:ASP:HB2 | 1:A:94:ARG:HG2 | 7 | 0.25 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 2 | 0.25 |
| (1,1654) | 1:A:134:ILE:H | 1:A:127:ARG:HB2 | 4 | 0.25 |
| (1,1634) | 1:A:131:HIS:H | 1:A:129:ASP:HB3 | 1 | 0.25 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD1 | 10 | 0.25 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD2 | 10 | 0.25 |
| (1,1591) | 1:A:126:GLU:H | 1:A:135:SER:HB2 | 8 | 0.25 |
| (1,1591) | 1:A:126:GLU:H | 1:A:135:SER:HB3 | 8 | 0.25 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB1 | 6 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB2 | 6 | 0.25 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB3 | 6 | 0.25 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 3 | 0.25 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 3 | 0.25 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 7 | 0.25 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 7 | 0.25 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 3 | 0.25 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 3 | 0.25 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 3 | 0.25 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 6 | 0.25 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD21 | 5 | 0.25 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD22 | 5 | 0.25 |
| (1,1372) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD23 | 5 | 0.25 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG21 | 3 | 0.25 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG22 | 3 | 0.25 |
| (1,1344) | 1:A:97:VAL:H | 1:A:165:VAL:HG23 | 3 | 0.25 |
| (1,1327) | 1:A:94:ARG:H | 1:A:169:MET:HG2 | 6 | 0.25 |
| (1,1210) | 1:A:160:GLU:HB2 | 1:A:162:THR:HB | 9 | 0.25 |
| (1,1173) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB3 | 9 | 0.25 |
| (1,1173) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB3 | 9 | 0.25 |
| (1,1173) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB3 | 9 | 0.25 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 3 | 0.25 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 3 | 0.25 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 10 | 0.25 |
| (1,102) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HB3 | 5 | 0.25 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 2 | 0.24 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 2 | 0.24 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 2 | 0.24 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 8 | 0.24 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 8 | 0.24 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 8 | 0.24 |
| (1,862) | 1:A:141:LYS:HG3 | 1:A:142:TYR:HB3 | 9 | 0.24 |
| (1,858) | 1:A:141:LYS:HG3 | 1:A:141:LYS:HE2 | 5 | 0.24 |
| (1,79) | 1:A:96:ARG:HA | 1:A:96:ARG:HG3 | 3 | 0.24 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE1 | 5 | 0.24 |
| (1,754) | 1:A:128:GLN:HB2 | 1:A:133:TYR:HE2 | 5 | 0.24 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 7 | 0.24 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 7 | 0.24 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 7 | 0.24 |
| (1,654) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HD2 | 7 | 0.24 |
| (1,654) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HD2 | 7 | 0.24 |
| (1,654) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HD2 | 7 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG21 | 8 | 0.24 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG22 | 8 | 0.24 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG23 | 8 | 0.24 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG21 | 10 | 0.24 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG22 | 10 | 0.24 |
| (1,638) | 1:A:120:ILE:HG12 | 1:A:120:ILE:HG23 | 10 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 2 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 8 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 8 | 0.24 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 8 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 8 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 8 | 0.24 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 8 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 8 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 8 | 0.24 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 8 | 0.24 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 1 | 0.24 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 1 | 0.24 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 1 | 0.24 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 1 | 0.24 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 1 | 0.24 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 1 | 0.24 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 8 | 0.24 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 8 | 0.24 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 8 | 0.24 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 8 | 0.24 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 8 | 0.24 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 8 | 0.24 |
| (1,528) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HB | 8 | 0.24 |
| (1,51) | 1:A:95:TRP:HA | 1:A:95:TRP:HB2 | 10 | 0.24 |
| (1,434) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG12 | 7 | 0.24 |
| (1,434) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG12 | 7 | 0.24 |
| (1,434) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG12 | 7 | 0.24 |
| (1,434) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG12 | 7 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,434) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG12 | 7 | 0.24 |
| (1,434) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG12 | 7 | 0.24 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD2 | 5 | 0.24 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD3 | 5 | 0.24 |
| (1,4262) | 1:B:167:ALA:H | 1:B:166:GLU:HB2 | 10 | 0.24 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 7 | 0.24 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 7 | 0.24 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 7 | 0.24 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 7 | 0.24 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 7 | 0.24 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 7 | 0.24 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG21 | 1 | 0.24 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG22 | 1 | 0.24 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG23 | 1 | 0.24 |
| (1,4128) | 1:B:155:SER:H | 1:B:154:SER:HB2 | 3 | 0.24 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 2 | 0.24 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 2 | 0.24 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 2 | 0.24 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 2 | 0.24 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 2 | 0.24 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 2 | 0.24 |
| (1,3910) | 1:B:129:ASP:H | 1:B:133:TYR:HB2 | 1 | 0.24 |
| (1,3865) | 1:B:125:GLU:H | 1:B:126:GLU:H | 4 | 0.24 |
| (1,3865) | 1:B:125:GLU:H | 1:B:126:GLU:H | 9 | 0.24 |
| (1,3848) | 1:B:123:LYS:H | 1:B:109:LEU:HG | 4 | 0.24 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 9 | 0.24 |
| (1,373) | 1:A:109:LEU:HD11 | 1:A:161:GLY:HA3 | 6 | 0.24 |
| (1,373) | 1:A:109:LEU:HD12 | 1:A:161:GLY:HA3 | 6 | 0.24 |
| (1,373) | 1:A:109:LEU:HD13 | 1:A:161:GLY:HA3 | 6 | 0.24 |
| (1,3726) | 1:B:111:VAL:H | 1:B:110:THR:HB | 10 | 0.24 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 6 | 0.24 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 8 | 0.24 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 8 | 0.24 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 8 | 0.24 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 8 | 0.24 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 8 | 0.24 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 8 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 1 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 1 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 1 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 2 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 2 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 2 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 7 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 7 | 0.24 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 7 | 0.24 |
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG21 | 1 | 0.24 |
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG22 | 1 | 0.24 |
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG23 | 1 | 0.24 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 1 | 0.24 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 1 | 0.24 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 5 | 0.24 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 5 | 0.24 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 5 | 0.24 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 5 | 0.24 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 5 | 0.24 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 5 | 0.24 |
| (1,3138) | 1:B:141:LYS:HG2 | 1:B:143:THR:HA | 4 | 0.24 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 6 | 0.24 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 3 | 0.24 |
| (1,3004) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB2 | 8 | 0.24 |
| (1,2996) | 1:B:126:GLU:HB2 | 1:B:135:SER:HB3 | 4 | 0.24 |
| (1,2996) | 1:B:126:GLU:HB3 | 1:B:135:SER:HB3 | 4 | 0.24 |
| (1,2991) | 1:B:126:GLU:HA | 1:B:135:SER:HB2 | 8 | 0.24 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 5 | 0.24 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 5 | 0.24 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 7 | 0.24 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 7 | 0.24 |
| (1,2918) | 1:B:120:ILE:HB | 1:B:142:TYR:HE1 | 9 | 0.24 |
| (1,2918) | 1:B:120:ILE:HB | 1:B:142:TYR:HE2 | 9 | 0.24 |
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 1 | 0.24 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 1 | 0.24 |
| (1,2738) | 1:B:112:LYS:HB2 | 1:B:120:ILE:HA | 10 | 0.24 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 6 | 0.24 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 6 | 0.24 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 6 | 0.24 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD11 | 9 | 0.24 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD12 | 9 | 0.24 |
| (1,2645) | 1:B:109:LEU:HG | 1:B:120:ILE:HD13 | 9 | 0.24 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 6 | 0.24 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 6 | 0.24 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 6 | 0.24 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 10 | 0.24 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 10 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 10 | 0.24 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 3 | 0.24 |
| (1,2625) | 1:B:108:GLU:HG2 | 1:B:123:LYS:HD3 | 4 | 0.24 |
| (1,2625) | 1:B:108:GLU:HG2 | 1:B:123:LYS:HD2 | 4 | 0.24 |
| (1,2617) | 1:B:108:GLU:HA | 1:B:108:GLU:HG2 | 4 | 0.24 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 2 | 0.24 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 2 | 0.24 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 2 | 0.24 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 5 | 0.24 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 5 | 0.24 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 5 | 0.24 |
| (1,247) | 1:A:99:LEU:HD21 | 1:A:140:ARG:HG3 | 4 | 0.24 |
| (1,247) | 1:A:99:LEU:HD22 | 1:A:140:ARG:HG3 | 4 | 0.24 |
| (1,247) | 1:A:99:LEU:HD23 | 1:A:140:ARG:HG3 | 4 | 0.24 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 7 | 0.24 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 7 | 0.24 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 7 | 0.24 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD3 | 3 | 0.24 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD2 | 3 | 0.24 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG21 | 5 | 0.24 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG22 | 5 | 0.24 |
| (1,2364) | 1:B:96:ARG:HA | 1:B:97:VAL:HG23 | 5 | 0.24 |
| (1,234) | 1:A:99:LEU:HD11 | 1:A:140:ARG:HD3 | 4 | 0.24 |
| (1,234) | 1:A:99:LEU:HD12 | 1:A:140:ARG:HD3 | 4 | 0.24 |
| (1,234) | 1:A:99:LEU:HD13 | 1:A:140:ARG:HD3 | 4 | 0.24 |
| (1,234) | 1:A:99:LEU:HD11 | 1:A:140:ARG:HD2 | 4 | 0.24 |
| (1,234) | 1:A:99:LEU:HD12 | 1:A:140:ARG:HD2 | 4 | 0.24 |
| (1,234) | 1:A:99:LEU:HD13 | 1:A:140:ARG:HD2 | 4 | 0.24 |
| (1,2322) | 1:B:94:ARG:HB3 | 1:B:167:ALA:HA | 9 | 0.24 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 5 | 0.24 |
| (1,2192) | 1:B:134:ILE:HA | 1:A:140:ARG:HG3 | 3 | 0.24 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 5 | 0.24 |
| (1,2060) | 1:B:134:ILE:HA | 1:A:140:ARG:HG3 | 3 | 0.24 |
| (1,20) | 1:A:93:ASP:HB3 | 1:A:94:ARG:HA | 5 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 4 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 4 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 6 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 6 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 7 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 7 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 8 | 0.24 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 8 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 6 | 0.24 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 10 | 0.24 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 10 | 0.24 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 10 | 0.24 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 10 | 0.24 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 10 | 0.24 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 10 | 0.24 |
| (1,1884) | 1:A:158:SER:H | 1:A:158:SER:HB3 | 2 | 0.24 |
| (1,1796) | 1:A:152:GLN:HE21 | 1:A:149:ASP:HB2 | 4 | 0.24 |
| (1,1796) | 1:A:152:GLN:HE21 | 1:A:149:ASP:HB2 | 8 | 0.24 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD1 | 2 | 0.24 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD2 | 2 | 0.24 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 10 | 0.24 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 10 | 0.24 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 10 | 0.24 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 10 | 0.24 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 10 | 0.24 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 10 | 0.24 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 2 | 0.24 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 4 | 0.24 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE2 | 3 | 0.24 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE2 | 3 | 0.24 |
| (1,1302) | 1:A:169:MET:HB2 | 1:A:171:LYS:HE3 | 3 | 0.24 |
| (1,1302) | 1:A:169:MET:HB3 | 1:A:171:LYS:HE3 | 3 | 0.24 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 5 | 0.24 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 5 | 0.24 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 5 | 0.24 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 6 | 0.24 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 6 | 0.24 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 6 | 0.24 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 5 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD21 | 1 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD22 | 1 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD23 | 1 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD21 | 6 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD22 | 6 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD23 | 6 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD21 | 8 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD22 | 8 | 0.24 |
| (1,1122) | 1:A:155:SER:HB3 | 1:A:157:LEU:HD23 | 8 | 0.24 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 8 | 0.24 |
| (1,1065) | 1:A:152:GLN:HB2 | 1:A:169:MET:HA | 8 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG21 | 1 | 0.23 |
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG22 | 1 | 0.23 |
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG23 | 1 | 0.23 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG21 | 1 | 0.23 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG22 | 1 | 0.23 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG23 | 1 | 0.23 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 5 | 0.23 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 6 | 0.23 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 6 | 0.23 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 6 | 0.23 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG21 | 9 | 0.23 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG22 | 9 | 0.23 |
| (1,83) | 1:A:96:ARG:HA | 1:A:97:VAL:HG23 | 9 | 0.23 |
| (1,827) | 1:A:139:THR:HA | 1:A:140:ARG:HG2 | 2 | 0.23 |
| (1,773) | 1:A:130:GLU:HA | 1:A:130:GLU:HG3 | 9 | 0.23 |
| (1,756) | 1:A:128:GLN:HB3 | 1:A:133:TYR:HD1 | 1 | 0.23 |
| (1,756) | 1:A:128:GLN:HB3 | 1:A:133:TYR:HD2 | 1 | 0.23 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 9 | 0.23 |
| (1,737) | 1:A:127:ARG:HA | 1:A:127:ARG:HD3 | 2 | 0.23 |
| (1,664) | 1:A:121:THR:HA | 1:A:139:THR:HA | 6 | 0.23 |
| (1,648) | 1:A:120:ILE:HG21 | 1:A:139:THR:HA | 5 | 0.23 |
| (1,648) | 1:A:120:ILE:HG22 | 1:A:139:THR:HA | 5 | 0.23 |
| (1,648) | 1:A:120:ILE:HG23 | 1:A:139:THR:HA | 5 | 0.23 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 1 | 0.23 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 4 | 0.23 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 6 | 0.23 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 6 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 6 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 6 | 0.23 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 6 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 6 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 6 | 0.23 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 6 | 0.23 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 10 | 0.23 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 10 | 0.23 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 10 | 0.23 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 4 | 0.23 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 4 | 0.23 |
| (1,474) | 1:A:112:LYS:HE3 | 1:A:114:LYS:HB3 | 5 | 0.23 |
| (1,474) | 1:A:112:LYS:HE2 | 1:A:114:LYS:HB3 | 5 | 0.23 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG21 | 2 | 0.23 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG22 | 2 | 0.23 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG23 | 2 | 0.23 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG2 | 4 | 0.23 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG3 | 4 | 0.23 |
| (1,4196) | 1:B:162:THR:H | 1:B:102:ASN:HB2 | 7 | 0.23 |
| (1,4052) | 1:B:151:THR:H | 1:B:149:ASP:HB3 | 1 | 0.23 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG11 | 9 | 0.23 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG12 | 9 | 0.23 |
| (1,4011) | 1:B:144:LEU:H | 1:B:148:VAL:HG13 | 9 | 0.23 |
| (1,3902) | 1:B:129:ASP:H | 1:B:129:ASP:HB2 | 9 | 0.23 |
| (1,3893) | 1:B:128:GLN:HE22 | 1:B:129:ASP:H | 6 | 0.23 |
| (1,3848) | 1:B:123:LYS:H | 1:B:109:LEU:HG | 7 | 0.23 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 3 | 0.23 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 3 | 0.23 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 3 | 0.23 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 10 | 0.23 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 10 | 0.23 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 10 | 0.23 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 10 | 0.23 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 10 | 0.23 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 10 | 0.23 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 10 | 0.23 |
| (1,3763) | 1:B:114:LYS:H | 1:B:115:ASP:HB2 | 5 | 0.23 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB2 | 7 | 0.23 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB3 | 7 | 0.23 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3664) | 1:B:102:ASN:HD22 | 1:B:161:GLY:HA3 | 3 | 0.23 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD11 | 4 | 0.23 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD12 | 4 | 0.23 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD13 | 4 | 0.23 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD11 | 5 | 0.23 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD12 | 5 | 0.23 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD13 | 5 | 0.23 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 1 | 0.23 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 10 | 0.23 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 5 | 0.23 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 5 | 0.23 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 5 | 0.23 |
| (1,3557) | 1:B:168:PRO:HA | 1:B:169:MET:HG2 | 3 | 0.23 |
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG21 | 9 | 0.23 |
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG22 | 9 | 0.23 |
| (1,3500) | 1:B:162:THR:HA | 1:B:162:THR:HG23 | 9 | 0.23 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 7 | 0.23 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 3 | 0.23 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 9 | 0.23 |
| (1,336) | 1:A:108:GLU:HA | 1:A:108:GLU:HG2 | 8 | 0.23 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 2 | 0.23 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 2 | 0.23 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 2 | 0.23 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 4 | 0.23 |
| (1,3295) | 1:B:148:VAL:HG11 | 1:B:170:PRO:HG3 | 7 | 0.23 |
| (1,3295) | 1:B:148:VAL:HG12 | 1:B:170:PRO:HG3 | 7 | 0.23 |
| (1,3295) | 1:B:148:VAL:HG13 | 1:B:170:PRO:HG3 | 7 | 0.23 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 4 | 0.23 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 4 | 0.23 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 4 | 0.23 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 4 | 0.23 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 4 | 0.23 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 4 | 0.23 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG11 | 8 | 0.23 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG12 | 8 | 0.23 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG13 | 8 | 0.23 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG11 | 8 | 0.23 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG12 | 8 | 0.23 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG13 | 8 | 0.23 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 7 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 1 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 1 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 1 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 1 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 1 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 1 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 1 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 1 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 1 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 4 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 6 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 6 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 6 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 6 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 6 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 6 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 6 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 6 | 0.23 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 6 | 0.23 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 4 | 0.23 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 4 | 0.23 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 4 | 0.23 |
| (1,3139) | 1:B:141:LYS:HG3 | 1:B:141:LYS:HE2 | 3 | 0.23 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 4 | 0.23 |
| (1,3116) | 1:B:139:THR:HG21 | 1:B:141:LYS:HE2 | 2 | 0.23 |
| (1,3116) | 1:B:139:THR:HG22 | 1:B:141:LYS:HE2 | 2 | 0.23 |
| (1,3116) | 1:B:139:THR:HG23 | 1:B:141:LYS:HE2 | 2 | 0.23 |
| (1,3003) | 1:B:126:GLU:HG2 | 1:B:135:SER:HA | 10 | 0.23 |
| (1,2982) | 1:B:125:GLU:HA | 1:B:126:GLU:HG2 | 4 | 0.23 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 3 | 0.23 |
| (1,2930) | 1:B:120:ILE:HG21 | 1:B:140:ARG:HA | 2 | 0.23 |
| (1,2930) | 1:B:120:ILE:HG22 | 1:B:140:ARG:HA | 2 | 0.23 |
| (1,2930) | 1:B:120:ILE:HG23 | 1:B:140:ARG:HA | 2 | 0.23 |
| (1,2929) | 1:B:120:ILE:HG21 | 1:B:139:THR:HA | 8 | 0.23 |
| (1,2929) | 1:B:120:ILE:HG22 | 1:B:139:THR:HA | 8 | 0.23 |
| (1,2929) | 1:B:120:ILE:HG23 | 1:B:139:THR:HA | 8 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 8 | 0.23 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 8 | 0.23 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 8 | 0.23 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG11 | 7 | 0.23 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG12 | 7 | 0.23 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG13 | 7 | 0.23 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 2 | 0.23 |
| (1,2776) | 1:B:113:THR:HG21 | 1:B:116:GLY:HA3 | 2 | 0.23 |
| (1,2776) | 1:B:113:THR:HG22 | 1:B:116:GLY:HA3 | 2 | 0.23 |
| (1,2776) | 1:B:113:THR:HG23 | 1:B:116:GLY:HA3 | 2 | 0.23 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 5 | 0.23 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 5 | 0.23 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 5 | 0.23 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 6 | 0.23 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 2 | 0.23 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 2 | 0.23 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 2 | 0.23 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 2 | 0.23 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 2 | 0.23 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 2 | 0.23 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 3 | 0.23 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 6 | 0.23 |
| (1,2560) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA2 | 10 | 0.23 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD21 | 9 | 0.23 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD22 | 9 | 0.23 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD23 | 9 | 0.23 |
| (1,2484) | 1:B:99:LEU:HA | 1:B:100:ASP:HB3 | 10 | 0.23 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 5 | 0.23 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 8 | 0.23 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 8 | 0.23 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 8 | 0.23 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD3 | 1 | 0.23 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD2 | 1 | 0.23 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 8 | 0.23 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 8 | 0.23 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 8 | 0.23 |
| (1,2332) | 1:B:95:TRP:HA | 1:B:95:TRP:HB2 | 1 | 0.23 |
| (1,2310) | 1:B:94:ARG:HA | 1:B:168:PRO:HA | 7 | 0.23 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 3 | 0.23 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 3 | 0.23 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 3 | 0.23 |
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD21 | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD22 | 6 | 0.23 |
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD23 | 6 | 0.23 |
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 1 | 0.23 |
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 3 | 0.23 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 1 | 0.23 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 5 | 0.23 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 5 | 0.23 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 5 | 0.23 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 6 | 0.23 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 6 | 0.23 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 6 | 0.23 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 6 | 0.23 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 6 | 0.23 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 6 | 0.23 |
| (1,1675) | 1:A:137:CYS:H | 1:A:136:ARG:HG2 | 4 | 0.23 |
| (1,1655) | 1:A:134:ILE:H | 1:A:127:ARG:HG2 | 7 | 0.23 |
| (1,1650) | 1:A:132:GLY:H | 1:A:133:TYR:HD1 | 4 | 0.23 |
| (1,1650) | 1:A:132:GLY:H | 1:A:133:TYR:HD2 | 4 | 0.23 |
| (1,1637) | 1:A:131:HIS:H | 1:A:130:GLU:HG2 | 7 | 0.23 |
| (1,1637) | 1:A:131:HIS:H | 1:A:130:GLU:HG3 | 7 | 0.23 |
| (1,1637) | 1:A:131:HIS:H | 1:A:130:GLU:HG2 | 9 | 0.23 |
| (1,1637) | 1:A:131:HIS:H | 1:A:130:GLU:HG3 | 9 | 0.23 |
| (1,1626) | 1:A:129:ASP:H | 1:A:132:GLY:HA3 | 2 | 0.23 |
| (1,1621) | 1:A:129:ASP:H | 1:A:129:ASP:HB2 | 2 | 0.23 |
| (1,1621) | 1:A:129:ASP:H | 1:A:129:ASP:HB2 | 5 | 0.23 |
| (1,1580) | 1:A:125:GLU:H | 1:A:108:GLU:HG2 | 5 | 0.23 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 10 | 0.23 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB2 | 5 | 0.23 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB3 | 5 | 0.23 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 8 | 0.23 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 8 | 0.23 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 8 | 0.23 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 5 | 0.23 |
| (1,1383) | 1:A:102:ASN:HD22 | 1:A:161:GLY:HA3 | 2 | 0.23 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD21 | 4 | 0.23 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD22 | 4 | 0.23 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD23 | 4 | 0.23 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD21 | 7 | 0.23 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD22 | 7 | 0.23 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD23 | 7 | 0.23 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB2 | 9 | 0.23 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB3 | 9 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 3 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 3 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 3 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 3 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 3 | 0.23 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 3 | 0.23 |
| (1,1321) | 1:A:94:ARG:H | 1:A:93:ASP:HA | 1 | 0.23 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 1 | 0.23 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 1 | 0.23 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 1 | 0.23 |
| (1,1289) | 1:A:169:MET:HA | 1:A:169:MET:HG3 | 8 | 0.23 |
| (1,1193) | 1:A:158:SER:HB3 | 1:A:160:GLU:HB3 | 10 | 0.23 |
| (1,1173) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB3 | 5 | 0.23 |
| (1,1173) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB3 | 5 | 0.23 |
| (1,1173) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB3 | 5 | 0.23 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 2 | 0.23 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 2 | 0.23 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 6 | 0.23 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 2 | 0.23 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 1 | 0.22 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 1 | 0.22 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 1 | 0.22 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 3 | 0.22 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 3 | 0.22 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 3 | 0.22 |
| (1,744) | 1:A:127:ARG:HB3 | 1:A:127:ARG:HD3 | 4 | 0.22 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 4 | 0.22 |
| (1,717) | 1:A:126:GLU:HG2 | 1:A:127:ARG:HG3 | 5 | 0.22 |
| (1,700) | 1:A:125:GLU:HA | 1:A:125:GLU:HG3 | 8 | 0.22 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 6 | 0.22 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 6 | 0.22 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 10 | 0.22 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 10 | 0.22 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 10 | 0.22 |
| (1,655) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HD3 | 6 | 0.22 |
| (1,655) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HD3 | 6 | 0.22 |
| (1,655) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HD3 | 6 | 0.22 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 1 | 0.22 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 1 | 0.22 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 1 | 0.22 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG11 | 6 | 0.22 |
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG12 | 6 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,62) | 1:A:95:TRP:HB2 | 1:A:148:VAL:HG13 | 6 | 0.22 |
| (1,61) | 1:A:95:TRP:HB2 | 1:A:96:ARG:HA | 4 | 0.22 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 2 | 0.22 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 2 | 0.22 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 2 | 0.22 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 2 | 0.22 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 2 | 0.22 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 2 | 0.22 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 5 | 0.22 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 5 | 0.22 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 5 | 0.22 |
| (1,502) | 1:A:113:THR:HG21 | 1:A:150:PRO:HB3 | 3 | 0.22 |
| (1,502) | 1:A:113:THR:HG22 | 1:A:150:PRO:HB3 | 3 | 0.22 |
| (1,502) | 1:A:113:THR:HG23 | 1:A:150:PRO:HB3 | 3 | 0.22 |
| (1,494) | 1:A:113:THR:HG21 | 1:A:116:GLY:HA2 | 5 | 0.22 |
| (1,494) | 1:A:113:THR:HG22 | 1:A:116:GLY:HA2 | 5 | 0.22 |
| (1,494) | 1:A:113:THR:HG23 | 1:A:116:GLY:HA2 | 5 | 0.22 |
| (1,457) | 1:A:112:LYS:HB2 | 1:A:120:ILE:HA | 8 | 0.22 |
| (1,457) | 1:A:112:LYS:HB2 | 1:A:120:ILE:HA | 9 | 0.22 |
| (1,44) | 1:A:94:ARG:HG2 | 1:A:166:GLU:HB2 | 10 | 0.22 |
| (1,44) | 1:A:94:ARG:HG3 | 1:A:166:GLU:HB2 | 10 | 0.22 |
| (1,4290) | 1:B:171:LYS:H | 1:B:171:LYS:HB2 | 5 | 0.22 |
| (1,4290) | 1:B:171:LYS:H | 1:B:171:LYS:HB3 | 5 | 0.22 |
| (1,4282) | 1:B:169:MET:H | 1:B:170:PRO:HD2 | 5 | 0.22 |
| (1,4282) | 1:B:169:MET:H | 1:B:170:PRO:HD3 | 5 | 0.22 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG21 | 8 | 0.22 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG22 | 8 | 0.22 |
| (1,4273) | 1:B:169:MET:H | 1:B:148:VAL:HG23 | 8 | 0.22 |
| (1,4263) | 1:B:167:ALA:H | 1:B:166:GLU:HB3 | 5 | 0.22 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 5 | 0.22 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 8 | 0.22 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 4 | 0.22 |
| (1,4052) | 1:B:151:THR:H | 1:B:149:ASP:HB3 | 3 | 0.22 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 1 | 0.22 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 1 | 0.22 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 1 | 0.22 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 2 | 0.22 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 2 | 0.22 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 2 | 0.22 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD11 | 8 | 0.22 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD12 | 8 | 0.22 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD13 | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD21 | 8 | 0.22 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD22 | 8 | 0.22 |
| (1,3971) | 1:B:140:ARG:H | 1:B:99:LEU:HD23 | 8 | 0.22 |
| (1,3955) | 1:B:137:CYS:H | 1:B:136:ARG:HB3 | 1 | 0.22 |
| (1,3955) | 1:B:137:CYS:H | 1:B:136:ARG:HB3 | 6 | 0.22 |
| (1,3908) | 1:B:129:ASP:H | 1:B:132:GLY:H | 8 | 0.22 |
| (1,3872) | 1:B:126:GLU:H | 1:B:135:SER:HB2 | 1 | 0.22 |
| (1,3872) | 1:B:126:GLU:H | 1:B:135:SER:HB3 | 1 | 0.22 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB2 | 5 | 0.22 |
| (1,3867) | 1:B:126:GLU:H | 1:B:125:GLU:HB3 | 5 | 0.22 |
| (1,3861) | 1:B:125:GLU:H | 1:B:108:GLU:HG2 | 1 | 0.22 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 5 | 0.22 |
| (1,3795) | 1:B:118:VAL:H | 1:B:119:GLU:HG3 | 1 | 0.22 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 1 | 0.22 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 7 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 1 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 1 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 1 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 1 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 1 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 1 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 5 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 5 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 5 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 5 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 5 | 0.22 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 5 | 0.22 |
| (1,3699) | 1:B:108:GLU:H | 1:B:108:GLU:HG2 | 4 | 0.22 |
| (1,3699) | 1:B:108:GLU:H | 1:B:108:GLU:HG3 | 4 | 0.22 |
| (1,3680) | 1:B:107:ASP:H | 1:B:106:PRO:HB2 | 7 | 0.22 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD11 | 6 | 0.22 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD12 | 6 | 0.22 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD13 | 6 | 0.22 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 4 | 0.22 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 4 | 0.22 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 4 | 0.22 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 4 | 0.22 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 4 | 0.22 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 4 | 0.22 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG21 | 2 | 0.22 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG22 | 2 | 0.22 |
| (1,3625) | 1:B:97:VAL:H | 1:B:165:VAL:HG23 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3604) | 1:B:94:ARG:H | 1:B:93:ASP:HB3 | 10 | 0.22 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 3 | 0.22 |
| (1,3584) | 1:B:169:MET:HG2 | 1:B:170:PRO:HD2 | 7 | 0.22 |
| (1,3584) | 1:B:169:MET:HG2 | 1:B:170:PRO:HD3 | 7 | 0.22 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 4 | 0.22 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 4 | 0.22 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 4 | 0.22 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 8 | 0.22 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 8 | 0.22 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 8 | 0.22 |
| (1,3539) | 1:B:166:GLU:HG2 | 1:B:167:ALA:HA | 5 | 0.22 |
| (1,3539) | 1:B:166:GLU:HG3 | 1:B:167:ALA:HA | 5 | 0.22 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 2 | 0.22 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 3 | 0.22 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 8 | 0.22 |
| (1,3473) | 1:B:158:SER:HB2 | 1:B:162:THR:HB | 3 | 0.22 |
| (1,3436) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HA | 6 | 0.22 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 6 | 0.22 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 7 | 0.22 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 7 | 0.22 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 7 | 0.22 |
| (1,3319) | 1:B:150:PRO:HB2 | 1:B:150:PRO:HD2 | 9 | 0.22 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 2 | 0.22 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 10 | 0.22 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 6 | 0.22 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 6 | 0.22 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 6 | 0.22 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 1 | 0.22 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 1 | 0.22 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 1 | 0.22 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 6 | 0.22 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 6 | 0.22 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 6 | 0.22 |
| (1,3139) | 1:B:141:LYS:HG3 | 1:B:141:LYS:HE2 | 4 | 0.22 |
| (1,3137) | 1:B:141:LYS:HG2 | 1:B:142:TYR:HB3 | 4 | 0.22 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 2 | 0.22 |
| (1,3028) | 1:B:128:GLN:HA | 1:B:133:TYR:HB2 | 7 | 0.22 |
| (1,3005) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB3 | 5 | 0.22 |
| (1,2986) | 1:B:126:GLU:HA | 1:B:126:GLU:HG3 | 8 | 0.22 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 8 | 0.22 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 8 | 0.22 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 9 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 9 | 0.22 |
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 4 | 0.22 |
| (1,2965) | 1:B:123:LYS:HA | 1:B:135:SER:HB3 | 1 | 0.22 |
| (1,2945) | 1:B:121:THR:HA | 1:B:139:THR:HA | 2 | 0.22 |
| (1,2929) | 1:B:120:ILE:HG21 | 1:B:139:THR:HA | 9 | 0.22 |
| (1,2929) | 1:B:120:ILE:HG22 | 1:B:139:THR:HA | 9 | 0.22 |
| (1,2929) | 1:B:120:ILE:HG23 | 1:B:139:THR:HA | 9 | 0.22 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG21 | 4 | 0.22 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG22 | 4 | 0.22 |
| (1,2922) | 1:B:120:ILE:HG13 | 1:B:120:ILE:HG23 | 4 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 5 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 9 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 9 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 9 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 9 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 9 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 9 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 9 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 9 | 0.22 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 9 | 0.22 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 5 | 0.22 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 5 | 0.22 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 5 | 0.22 |
| (1,2790) | 1:B:114:LYS:HA | 1:B:114:LYS:HB2 | 6 | 0.22 |
| (1,279) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA2 | 7 | 0.22 |
| (1,2783) | 1:B:113:THR:HG21 | 1:B:150:PRO:HB3 | 5 | 0.22 |
| (1,2783) | 1:B:113:THR:HG22 | 1:B:150:PRO:HB3 | 5 | 0.22 |
| (1,2783) | 1:B:113:THR:HG23 | 1:B:150:PRO:HB3 | 5 | 0.22 |
| (1,2783) | 1:B:113:THR:HG21 | 1:B:150:PRO:HB3 | 6 | 0.22 |
| (1,2783) | 1:B:113:THR:HG22 | 1:B:150:PRO:HB3 | 6 | 0.22 |
| (1,2783) | 1:B:113:THR:HG23 | 1:B:150:PRO:HB3 | 6 | 0.22 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 3 | 0.22 |
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 3 | 0.22 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 3 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 3 | 0.22 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 3 | 0.22 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD11 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD12 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HD13 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD11 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD12 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HD13 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD11 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD12 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HD13 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD11 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD12 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HD13 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD11 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD12 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HD13 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD11 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 3 | 0.22 |
| (1,2717) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HD13 | 3 | 0.22 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 2 | 0.22 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 2 | 0.22 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 2 | 0.22 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 10 | 0.22 |
| (1,2578) | 1:B:105:ALA:HB1 | 1:B:107:ASP:HB3 | 6 | 0.22 |
| (1,2578) | 1:B:105:ALA:HB2 | 1:B:107:ASP:HB3 | 6 | 0.22 |
| (1,2578) | 1:B:105:ALA:HB3 | 1:B:107:ASP:HB3 | 6 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG11 | 1:B:120:ILE:HD11 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG11 | 1:B:120:ILE:HD12 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG11 | 1:B:120:ILE:HD13 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG12 | 1:B:120:ILE:HD11 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG12 | 1:B:120:ILE:HD12 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG12 | 1:B:120:ILE:HD13 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG13 | 1:B:120:ILE:HD11 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG13 | 1:B:120:ILE:HD12 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG13 | 1:B:120:ILE:HD13 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG21 | 1:B:120:ILE:HD11 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG21 | 1:B:120:ILE:HD12 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG21 | 1:B:120:ILE:HD13 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG22 | 1:B:120:ILE:HD11 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG22 | 1:B:120:ILE:HD12 | 4 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2553) | 1:B:101:VAL:HG22 | 1:B:120:ILE:HD13 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG23 | 1:B:120:ILE:HD11 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG23 | 1:B:120:ILE:HD12 | 4 | 0.22 |
| (1,2553) | 1:B:101:VAL:HG23 | 1:B:120:ILE:HD13 | 4 | 0.22 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD1 | 10 | 0.22 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD2 | 10 | 0.22 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD1 | 10 | 0.22 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD2 | 10 | 0.22 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD1 | 10 | 0.22 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD2 | 10 | 0.22 |
| (1,2282) | 1:B:88:ILE:HG21 | 1:B:90:HIS:HA | 8 | 0.22 |
| (1,2282) | 1:B:88:ILE:HG22 | 1:B:90:HIS:HA | 8 | 0.22 |
| (1,2282) | 1:B:88:ILE:HG23 | 1:B:90:HIS:HA | 8 | 0.22 |
| (1,2169) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 8 | 0.22 |
| (1,2037) | 1:A:132:GLY:HA3 | 1:B:140:ARG:HB3 | 8 | 0.22 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 10 | 0.22 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 10 | 0.22 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 6 | 0.22 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 9 | 0.22 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 9 | 0.22 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 9 | 0.22 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 9 | 0.22 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 9 | 0.22 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 9 | 0.22 |
| (1,1902) | 1:A:161:GLY:H | 1:A:102:ASN:HB3 | 3 | 0.22 |
| (1,1844) | 1:A:154:SER:H | 1:A:168:PRO:HD2 | 7 | 0.22 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 2 | 0.22 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 2 | 0.22 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 2 | 0.22 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD2 | 4 | 0.22 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD3 | 4 | 0.22 |
| (1,1615) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HB3 | 7 | 0.22 |
| (1,1602) | 1:A:128:GLN:H | 1:A:128:GLN:HB3 | 7 | 0.22 |
| (1,1598) | 1:A:128:GLN:H | 1:A:127:ARG:HG2 | 1 | 0.22 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 7 | 0.22 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 7 | 0.22 |
| (1,1581) | 1:A:125:GLU:H | 1:A:108:GLU:HG3 | 8 | 0.22 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG21 | 4 | 0.22 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG22 | 4 | 0.22 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG23 | 4 | 0.22 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG11 | 4 | 0.22 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG12 | 4 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG13 | 4 | 0.22 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 8 | 0.22 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 9 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 3 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 3 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 3 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 3 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 3 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 3 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 8 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 8 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 8 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 8 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 8 | 0.22 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 8 | 0.22 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 4 | 0.22 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 1 | 0.22 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 6 | 0.22 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 9 | 0.22 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD11 | 7 | 0.22 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD12 | 7 | 0.22 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD13 | 7 | 0.22 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB2 | 7 | 0.22 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB3 | 7 | 0.22 |
| (1,1327) | 1:A:94:ARG:H | 1:A:169:MET:HG2 | 9 | 0.22 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 3 | 0.22 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 3 | 0.22 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 3 | 0.22 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 4 | 0.22 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 4 | 0.22 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 4 | 0.22 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 8 | 0.22 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 7 | 0.22 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 7 | 0.22 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 7 | 0.22 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 10 | 0.22 |
| (1,1114) | 1:A:155:SER:HB2 | 1:A:163:LEU:HA | 8 | 0.22 |
| (1,1097) | 1:A:154:SER:HB3 | 1:A:155:SER:HA | 10 | 0.22 |
| (1,1085) | 1:A:153:VAL:HG11 | 1:A:155:SER:HB3 | 2 | 0.22 |
| (1,1085) | 1:A:153:VAL:HG12 | 1:A:155:SER:HB3 | 2 | 0.22 |
| (1,1085) | 1:A:153:VAL:HG13 | 1:A:155:SER:HB3 | 2 | 0.22 |
| (1,1085) | 1:A:153:VAL:HG21 | 1:A:155:SER:HB3 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1085) | 1:A:153:VAL:HG22 | 1:A:155:SER:HB3 | 2 | 0.22 |
| (1,1085) | 1:A:153:VAL:HG23 | 1:A:155:SER:HB3 | 2 | 0.22 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 1 | 0.22 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 1 | 0.22 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 9 | 0.22 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 2 | 0.22 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 5 | 0.22 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 8 | 0.22 |
| (1,1014) | 1:A:148:VAL:HG11 | 1:A:170:PRO:HG3 | 9 | 0.22 |
| (1,1014) | 1:A:148:VAL:HG12 | 1:A:170:PRO:HG3 | 9 | 0.22 |
| (1,1014) | 1:A:148:VAL:HG13 | 1:A:170:PRO:HG3 | 9 | 0.22 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 1 | 0.21 |
| (1,93) | 1:A:96:ARG:HB2 | 1:A:96:ARG:HD3 | 4 | 0.21 |
| (1,93) | 1:A:96:ARG:HB2 | 1:A:96:ARG:HD2 | 4 | 0.21 |
| (1,93) | 1:A:96:ARG:HB2 | 1:A:96:ARG:HD3 | 8 | 0.21 |
| (1,93) | 1:A:96:ARG:HB2 | 1:A:96:ARG:HD2 | 8 | 0.21 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 7 | 0.21 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 7 | 0.21 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 7 | 0.21 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 4 | 0.21 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 8 | 0.21 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 9 | 0.21 |
| (1,827) | 1:A:139:THR:HA | 1:A:140:ARG:HG2 | 7 | 0.21 |
| (1,737) | 1:A:127:ARG:HA | 1:A:127:ARG:HD3 | 6 | 0.21 |
| (1,736) | 1:A:127:ARG:HA | 1:A:127:ARG:HG3 | 7 | 0.21 |
| (1,725) | 1:A:126:GLU:HG2 | 1:A:127:ARG:HA | 7 | 0.21 |
| (1,725) | 1:A:126:GLU:HG3 | 1:A:127:ARG:HA | 7 | 0.21 |
| (1,710) | 1:A:126:GLU:HA | 1:A:135:SER:HB2 | 6 | 0.21 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 2 | 0.21 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 2 | 0.21 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 5 | 0.21 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 5 | 0.21 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 5 | 0.21 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG21 | 3 | 0.21 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG22 | 3 | 0.21 |
| (1,641) | 1:A:120:ILE:HG13 | 1:A:120:ILE:HG23 | 3 | 0.21 |
| (1,612) | 1:A:119:GLU:HA | 1:A:141:LYS:HE3 | 6 | 0.21 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD21 | 9 | 0.21 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD22 | 9 | 0.21 |
| (1,588) | 1:A:118:VAL:HG11 | 1:A:144:LEU:HD23 | 9 | 0.21 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD21 | 9 | 0.21 |
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD22 | 9 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,588) | 1:A:118:VAL:HG12 | 1:A:144:LEU:HD23 | 9 | 0.21 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD21 | 9 | 0.21 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD22 | 9 | 0.21 |
| (1,588) | 1:A:118:VAL:HG13 | 1:A:144:LEU:HD23 | 9 | 0.21 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 9 | 0.21 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 9 | 0.21 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 9 | 0.21 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 9 | 0.21 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 9 | 0.21 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 9 | 0.21 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 3 | 0.21 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 3 | 0.21 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 3 | 0.21 |
| (1,475) | 1:A:112:LYS:HE2 | 1:A:119:GLU:HG2 | 7 | 0.21 |
| (1,475) | 1:A:112:LYS:HE3 | 1:A:119:GLU:HG2 | 7 | 0.21 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 1 | 0.21 |
| (1,434) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HG12 | 6 | 0.21 |
| (1,434) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HG12 | 6 | 0.21 |
| (1,434) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HG12 | 6 | 0.21 |
| (1,434) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HG12 | 6 | 0.21 |
| (1,434) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HG12 | 6 | 0.21 |
| (1,434) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HG12 | 6 | 0.21 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 5 | 0.21 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 5 | 0.21 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 5 | 0.21 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 5 | 0.21 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 5 | 0.21 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 5 | 0.21 |
| (1,4182) | 1:B:161:GLY:H | 1:B:102:ASN:HB2 | 6 | 0.21 |
| (1,4128) | 1:B:155:SER:H | 1:B:154:SER:HB2 | 8 | 0.21 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 9 | 0.21 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 9 | 0.21 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 9 | 0.21 |
| (1,404) | 1:A:110:THR:HG21 | 1:A:112:LYS:HB2 | 9 | 0.21 |
| (1,404) | 1:A:110:THR:HG22 | 1:A:112:LYS:HB2 | 9 | 0.21 |
| (1,404) | 1:A:110:THR:HG23 | 1:A:112:LYS:HB2 | 9 | 0.21 |
| (1,4034) | 1:B:148:VAL:H | 1:B:149:ASP:H | 5 | 0.21 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 7 | 0.21 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 7 | 0.21 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 7 | 0.21 |
| (1,4) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB3 | 5 | 0.21 |
| (1,4) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB3 | 5 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB2 | 7 | 0.21 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB3 | 7 | 0.21 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 6 | 0.21 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 6 | 0.21 |
| (1,3894) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HA | 8 | 0.21 |
| (1,3861) | 1:B:125:GLU:H | 1:B:108:GLU:HG2 | 2 | 0.21 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 9 | 0.21 |
| (1,3795) | 1:B:118:VAL:H | 1:B:119:GLU:HG3 | 10 | 0.21 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD21 | 4 | 0.21 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD22 | 4 | 0.21 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD23 | 4 | 0.21 |
| (1,3664) | 1:B:102:ASN:HD22 | 1:B:161:GLY:HA3 | 8 | 0.21 |
| (1,3663) | 1:B:102:ASN:HD22 | 1:B:161:GLY:HA2 | 5 | 0.21 |
| (1,3654) | 1:B:102:ASN:HD21 | 1:B:161:GLY:HA2 | 3 | 0.21 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD11 | 5 | 0.21 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD12 | 5 | 0.21 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD13 | 5 | 0.21 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 9 | 0.21 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 5 | 0.21 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 9 | 0.21 |
| (1,3481) | 1:B:159:PRO:HA | 1:B:159:PRO:HG3 | 7 | 0.21 |
| (1,3458) | 1:B:157:LEU:HD21 | 1:B:161:GLY:HA3 | 8 | 0.21 |
| (1,3458) | 1:B:157:LEU:HD22 | 1:B:161:GLY:HA3 | 8 | 0.21 |
| (1,3458) | 1:B:157:LEU:HD23 | 1:B:161:GLY:HA3 | 8 | 0.21 |
| (1,345) | 1:A:108:GLU:HG2 | 1:A:123:LYS:HE3 | 3 | 0.21 |
| (1,345) | 1:A:108:GLU:HG2 | 1:A:123:LYS:HE2 | 3 | 0.21 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 10 | 0.21 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 10 | 0.21 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 10 | 0.21 |
| (1,3430) | 1:B:157:LEU:HA | 1:B:163:LEU:HB3 | 9 | 0.21 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 8 | 0.21 |
| (1,3358) | 1:B:153:VAL:HA | 1:B:168:PRO:HD2 | 10 | 0.21 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 3 | 0.21 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 3 | 0.21 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 3 | 0.21 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG21 | 3 | 0.21 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG22 | 3 | 0.21 |
| (1,3327) | 1:B:150:PRO:HD2 | 1:B:151:THR:HG23 | 3 | 0.21 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 5 | 0.21 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 7 | 0.21 |
| (1,3288) | 1:B:148:VAL:HG11 | 1:B:153:VAL:HA | 2 | 0.21 |
| (1,3288) | 1:B:148:VAL:HG12 | 1:B:153:VAL:HA | 2 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3288) | 1:B:148:VAL:HG13 | 1:B:153:VAL:HA | 2 | 0.21 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 6 | 0.21 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 6 | 0.21 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 6 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 2 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 5 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 5 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 5 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 5 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 5 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 5 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 5 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 5 | 0.21 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 5 | 0.21 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 7 | 0.21 |
| (1,3108) | 1:B:139:THR:HA | 1:B:140:ARG:HG2 | 9 | 0.21 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 7 | 0.21 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 3 | 0.21 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 10 | 0.21 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE1 | 2 | 0.21 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE2 | 2 | 0.21 |
| (1,3015) | 1:B:127:ARG:HA | 1:B:127:ARG:HB3 | 7 | 0.21 |
| (1,3010) | 1:B:126:GLU:HG3 | 1:B:133:TYR:HB3 | 7 | 0.21 |
| (1,2999) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HB3 | 1 | 0.21 |
| (1,2984) | 1:B:125:GLU:HA | 1:B:135:SER:HB2 | 1 | 0.21 |
| (1,2981) | 1:B:125:GLU:HA | 1:B:125:GLU:HG3 | 2 | 0.21 |
| (1,2976) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HB2 | 2 | 0.21 |
| (1,2976) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HB2 | 2 | 0.21 |
| (1,2973) | 1:B:123:LYS:HG3 | 1:B:137:CYS:HB2 | 10 | 0.21 |
| (1,2945) | 1:B:121:THR:HA | 1:B:139:THR:HA | 3 | 0.21 |
| (1,2928) | 1:B:120:ILE:HG21 | 1:B:122:GLY:HA3 | 9 | 0.21 |
| (1,2928) | 1:B:120:ILE:HG22 | 1:B:122:GLY:HA3 | 9 | 0.21 |
| (1,2928) | 1:B:120:ILE:HG23 | 1:B:122:GLY:HA3 | 9 | 0.21 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 2 | 0.21 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 6 | 0.21 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 8 | 0.21 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG11 | 3 | 0.21 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG12 | 3 | 0.21 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG13 | 3 | 0.21 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG21 | 9 | 0.21 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG22 | 9 | 0.21 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG23 | 9 | 0.21 |
| (1,2791) | 1:B:114:LYS:HB2 | 1:B:118:VAL:HA | 2 | 0.21 |
| (1,2791) | 1:B:114:LYS:HB3 | 1:B:118:VAL:HA | 2 | 0.21 |
| (1,279) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA2 | 9 | 0.21 |
| (1,2756) | 1:B:112:LYS:HE2 | 1:B:119:GLU:HG2 | 6 | 0.21 |
| (1,2756) | 1:B:112:LYS:HE3 | 1:B:119:GLU:HG2 | 6 | 0.21 |
| (1,2738) | 1:B:112:LYS:HB2 | 1:B:120:ILE:HA | 9 | 0.21 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 5 | 0.21 |
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 5 | 0.21 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 5 | 0.21 |
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 5 | 0.21 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 5 | 0.21 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 5 | 0.21 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD11 | 6 | 0.21 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD12 | 6 | 0.21 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD13 | 6 | 0.21 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD21 | 6 | 0.21 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD22 | 6 | 0.21 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD23 | 6 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 2 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 2 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 2 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 2 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 2 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 2 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 2 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 2 | 0.21 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 2 | 0.21 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 4 | 0.21 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 4 | 0.21 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 4 | 0.21 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 8 | 0.21 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 8 | 0.21 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 8 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 2 | 0.21 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 1 | 0.21 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 1 | 0.21 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 1 | 0.21 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 1 | 0.21 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 1 | 0.21 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 1 | 0.21 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 8 | 0.21 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 10 | 0.21 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 8 | 0.21 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 8 | 0.21 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 8 | 0.21 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 2 | 0.21 |
| (1,2560) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA2 | 8 | 0.21 |
| (1,2559) | 1:B:102:ASN:HB2 | 1:B:161:GLY:HA3 | 5 | 0.21 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD21 | 3 | 0.21 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD22 | 3 | 0.21 |
| (1,2558) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD23 | 3 | 0.21 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD11 | 8 | 0.21 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD12 | 8 | 0.21 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD13 | 8 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG21 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG22 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG23 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG21 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG22 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG23 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG21 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG22 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG23 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG11 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG12 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG13 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG11 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG12 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG13 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG11 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG12 | 7 | 0.21 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG13 | 7 | 0.21 |
| (1,248) | 1:A:99:LEU:HD21 | 1:A:140:ARG:HD2 | 6 | 0.21 |
| (1,248) | 1:A:99:LEU:HD22 | 1:A:140:ARG:HD2 | 6 | 0.21 |
| (1,248) | 1:A:99:LEU:HD23 | 1:A:140:ARG:HD2 | 6 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 6 | 0.21 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 8 | 0.21 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 9 | 0.21 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 6 | 0.21 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 6 | 0.21 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 6 | 0.21 |
| (1,2341) | 1:B:95:TRP:HB2 | 1:B:95:TRP:HE3 | 10 | 0.21 |
| (1,2306) | 1:B:94:ARG:HA | 1:B:94:ARG:HG3 | 7 | 0.21 |
| (1,2212) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 3 | 0.21 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 5 | 0.21 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 5 | 0.21 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 5 | 0.21 |
| (1,2080) | 1:A:134:ILE:HA | 1:B:140:ARG:HD2 | 3 | 0.21 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD2 | 3 | 0.21 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD3 | 3 | 0.21 |
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 2 | 0.21 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 6 | 0.21 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 6 | 0.21 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 6 | 0.21 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 6 | 0.21 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 6 | 0.21 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 6 | 0.21 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG21 | 1 | 0.21 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG22 | 1 | 0.21 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG23 | 1 | 0.21 |
| (1,1816) | 1:A:153:VAL:H | 1:A:149:ASP:HB2 | 2 | 0.21 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 3 | 0.21 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 3 | 0.21 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 3 | 0.21 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 10 | 0.21 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 10 | 0.21 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 10 | 0.21 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 10 | 0.21 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 10 | 0.21 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 10 | 0.21 |
| (1,1653) | 1:A:132:GLY:H | 1:A:134:ILE:HG21 | 6 | 0.21 |
| (1,1653) | 1:A:132:GLY:H | 1:A:134:ILE:HG22 | 6 | 0.21 |
| (1,1653) | 1:A:132:GLY:H | 1:A:134:ILE:HG23 | 6 | 0.21 |
| (1,1647) | 1:A:132:GLY:H | 1:A:131:HIS:HB3 | 6 | 0.21 |
| (1,1647) | 1:A:132:GLY:H | 1:A:131:HIS:HB3 | 9 | 0.21 |
| (1,1626) | 1:A:129:ASP:H | 1:A:132:GLY:HA3 | 8 | 0.21 |
| (1,1621) | 1:A:129:ASP:H | 1:A:129:ASP:HB2 | 4 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 3 | 0.21 |
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 4 | 0.21 |
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 8 | 0.21 |
| (1,1611) | 1:A:128:GLN:HE22 | 1:A:128:GLN:H | 6 | 0.21 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 8 | 0.21 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 8 | 0.21 |
| (1,1580) | 1:A:125:GLU:H | 1:A:108:GLU:HG2 | 1 | 0.21 |
| (1,1545) | 1:A:120:ILE:H | 1:A:140:ARG:HG3 | 9 | 0.21 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD11 | 5 | 0.21 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD12 | 5 | 0.21 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD13 | 5 | 0.21 |
| (1,1517) | 1:A:118:VAL:H | 1:A:142:TYR:HB2 | 6 | 0.21 |
| (1,1514) | 1:A:118:VAL:H | 1:A:119:GLU:HG3 | 5 | 0.21 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 2 | 0.21 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 3 | 0.21 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB2 | 2 | 0.21 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB3 | 2 | 0.21 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 8 | 0.21 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 8 | 0.21 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 4 | 0.21 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 7 | 0.21 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD21 | 2 | 0.21 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD22 | 2 | 0.21 |
| (1,1381) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD23 | 2 | 0.21 |
| (1,1369) | 1:A:102:ASN:HD21 | 1:A:109:LEU:HD11 | 3 | 0.21 |
| (1,1369) | 1:A:102:ASN:HD21 | 1:A:109:LEU:HD12 | 3 | 0.21 |
| (1,1369) | 1:A:102:ASN:HD21 | 1:A:109:LEU:HD13 | 3 | 0.21 |
| (1,1326) | 1:A:94:ARG:H | 1:A:168:PRO:HA | 5 | 0.21 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 10 | 0.21 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 10 | 0.21 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 10 | 0.21 |
| (1,1258) | 1:A:166:GLU:HG2 | 1:A:167:ALA:HA | 2 | 0.21 |
| (1,1258) | 1:A:166:GLU:HG3 | 1:A:167:ALA:HA | 2 | 0.21 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG2 | 8 | 0.21 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG3 | 8 | 0.21 |
| (1,1210) | 1:A:160:GLU:HB2 | 1:A:162:THR:HB | 8 | 0.21 |
| (1,1193) | 1:A:158:SER:HB3 | 1:A:160:GLU:HB3 | 3 | 0.21 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 4 | 0.21 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 7 | 0.21 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 9 | 0.21 |
| (1,1038) | 1:A:150:PRO:HB2 | 1:A:150:PRO:HD2 | 7 | 0.21 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 4 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,967) | 1:A:146:PRO:HB3 | 1:A:147:GLY:HA2 | 10 | 0.2 |
| (1,96) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HB2 | 8 | 0.2 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 6 | 0.2 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 6 | 0.2 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 6 | 0.2 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 9 | 0.2 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 9 | 0.2 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 9 | 0.2 |
| (1,858) | 1:A:141:LYS:HG3 | 1:A:141:LYS:HE2 | 2 | 0.2 |
| (1,857) | 1:A:141:LYS:HG2 | 1:A:143:THR:HA | 8 | 0.2 |
| (1,849) | 1:A:141:LYS:HB2 | 1:A:141:LYS:HE2 | 1 | 0.2 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 3 | 0.2 |
| (1,815) | 1:A:136:ARG:HG3 | 1:A:138:PHE:HA | 6 | 0.2 |
| (1,773) | 1:A:130:GLU:HA | 1:A:130:GLU:HG3 | 7 | 0.2 |
| (1,749) | 1:A:128:GLN:HA | 1:A:133:TYR:HE1 | 6 | 0.2 |
| (1,749) | 1:A:128:GLN:HA | 1:A:133:TYR:HE2 | 6 | 0.2 |
| (1,746) | 1:A:128:GLN:HA | 1:A:128:GLN:HG3 | 9 | 0.2 |
| (1,746) | 1:A:128:GLN:HA | 1:A:128:GLN:HG3 | 10 | 0.2 |
| (1,705) | 1:A:126:GLU:HA | 1:A:126:GLU:HG3 | 10 | 0.2 |
| (1,700) | 1:A:125:GLU:HA | 1:A:125:GLU:HG3 | 6 | 0.2 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 2 | 0.2 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 2 | 0.2 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 2 | 0.2 |
| (1,635) | 1:A:120:ILE:HB | 1:A:140:ARG:HD2 | 8 | 0.2 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 3 | 0.2 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 3 | 0.2 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 3 | 0.2 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG21 | 10 | 0.2 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG22 | 10 | 0.2 |
| (1,514) | 1:A:115:ASP:HB2 | 1:A:143:THR:HG23 | 10 | 0.2 |
| (1,489) | 1:A:113:THR:HB | 1:A:150:PRO:HB2 | 4 | 0.2 |
| (1,465) | 1:A:112:LYS:HG2 | 1:A:118:VAL:HA | 1 | 0.2 |
| (1,465) | 1:A:112:LYS:HG3 | 1:A:118:VAL:HA | 1 | 0.2 |
| (1,4258) | 1:B:167:ALA:H | 1:B:96:ARG:HB2 | 8 | 0.2 |
| (1,4258) | 1:B:167:ALA:H | 1:B:96:ARG:HB3 | 8 | 0.2 |
| (1,4205) | 1:B:162:THR:H | 1:B:160:GLU:HB2 | 8 | 0.2 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG21 | 1 | 0.2 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG22 | 1 | 0.2 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG23 | 1 | 0.2 |
| (1,4183) | 1:B:161:GLY:H | 1:B:102:ASN:HB3 | 8 | 0.2 |
| (1,4182) | 1:B:161:GLY:H | 1:B:102:ASN:HB2 | 2 | 0.2 |
| (1,4141) | 1:B:156:SER:H | 1:B:157:LEU:HB3 | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4115) | 1:B:154:SER:H | 1:B:155:SER:HB2 | 5 | 0.2 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 4 | 0.2 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 4 | 0.2 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 4 | 0.2 |
| (1,3894) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HA | 7 | 0.2 |
| (1,3868) | 1:B:126:GLU:H | 1:B:125:GLU:HG2 | 4 | 0.2 |
| (1,3847) | 1:B:123:LYS:H | 1:B:109:LEU:HB2 | 8 | 0.2 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 6 | 0.2 |
| (1,3806) | 1:B:119:GLU:H | 1:B:114:LYS:HB3 | 7 | 0.2 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 7 | 0.2 |
| (1,3795) | 1:B:118:VAL:H | 1:B:119:GLU:HG3 | 8 | 0.2 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 4 | 0.2 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 4 | 0.2 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 4 | 0.2 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 4 | 0.2 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 4 | 0.2 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 4 | 0.2 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 6 | 0.2 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 9 | 0.2 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 9 | 0.2 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 9 | 0.2 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 9 | 0.2 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 9 | 0.2 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 9 | 0.2 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 9 | 0.2 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 9 | 0.2 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 9 | 0.2 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 9 | 0.2 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 9 | 0.2 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 9 | 0.2 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 9 | 0.2 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 9 | 0.2 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 9 | 0.2 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3641) | 1:B:101:VAL:H | 1:B:100:ASP:HB2 | 1 | 0.2 |
| (1,3641) | 1:B:101:VAL:H | 1:B:100:ASP:HB3 | 1 | 0.2 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 3 | 0.2 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 3 | 0.2 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 3 | 0.2 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 6 | 0.2 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD3 | 9 | 0.2 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD2 | 9 | 0.2 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 2 | 0.2 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 10 | 0.2 |
| (1,3409) | 1:B:155:SER:HB3 | 1:B:157:LEU:HB3 | 7 | 0.2 |
| (1,3409) | 1:B:155:SER:HB2 | 1:B:157:LEU:HB3 | 7 | 0.2 |
| (1,3358) | 1:B:153:VAL:HA | 1:B:168:PRO:HD2 | 3 | 0.2 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 6 | 0.2 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 8 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 3 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 3 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 3 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 3 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 3 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 3 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 3 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 3 | 0.2 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 3 | 0.2 |
| (1,3133) | 1:B:141:LYS:HG2 | 1:B:141:LYS:HE2 | 5 | 0.2 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 1 | 0.2 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 8 | 0.2 |
| (1,3093) | 1:B:136:ARG:HA | 1:B:136:ARG:HD2 | 8 | 0.2 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 1 | 0.2 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 2 | 0.2 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 4 | 0.2 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 5 | 0.2 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 6 | 0.2 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 9 | 0.2 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD11 | 8 | 0.2 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD12 | 8 | 0.2 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD13 | 8 | 0.2 |
| (1,3018) | 1:B:127:ARG:HA | 1:B:127:ARG:HD3 | 3 | 0.2 |
| (1,2981) | 1:B:125:GLU:HA | 1:B:125:GLU:HG3 | 1 | 0.2 |
| (1,2891) | 1:B:119:GLU:HA | 1:B:141:LYS:HD3 | 10 | 0.2 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 7 | 0.2 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 7 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 7 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 4 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 4 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 4 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 4 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 4 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 4 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 4 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 4 | 0.2 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 4 | 0.2 |
| (1,2791) | 1:B:114:LYS:HB2 | 1:B:118:VAL:HA | 10 | 0.2 |
| (1,2791) | 1:B:114:LYS:HB3 | 1:B:118:VAL:HA | 10 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG12 | 5 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG12 | 5 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG12 | 5 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG12 | 5 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG12 | 5 | 0.2 |
| (1,2715) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG12 | 5 | 0.2 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 9 | 0.2 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 9 | 0.2 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 9 | 0.2 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 9 | 0.2 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 9 | 0.2 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 9 | 0.2 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 9 | 0.2 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 9 | 0.2 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 9 | 0.2 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 5 | 0.2 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 7 | 0.2 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 8 | 0.2 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 1 | 0.2 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 2 | 0.2 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 5 | 0.2 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 6 | 0.2 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 7 | 0.2 |
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 9 | 0.2 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 9 | 0.2 |
| (1,2561) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA3 | 2 | 0.2 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 6 | 0.2 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 6 | 0.2 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 6 | 0.2 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 8 | 0.2 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 8 | 0.2 |
| (1,2540) | 1:B:100:ASP:HA | 1:B:100:ASP:HB3 | 4 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG21 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG22 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG23 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG21 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG22 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG23 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG21 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG22 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG23 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG11 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG12 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG13 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG11 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG12 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG13 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG11 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG12 | 10 | 0.2 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG13 | 10 | 0.2 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD11 | 3 | 0.2 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD12 | 3 | 0.2 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD13 | 3 | 0.2 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 1 | 0.2 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 1 | 0.2 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 1 | 0.2 |
| (1,2383) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HB3 | 5 | 0.2 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG21 | 3 | 0.2 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG22 | 3 | 0.2 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG23 | 3 | 0.2 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG21 | 8 | 0.2 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG22 | 8 | 0.2 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG23 | 8 | 0.2 |
| (1,23) | 1:A:94:ARG:HA | 1:A:94:ARG:HB3 | 6 | 0.2 |
| (1,2297) | 1:B:93:ASP:HA | 1:B:94:ARG:HD2 | 6 | 0.2 |
| (1,2281) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 7 | 0.2 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 1 | 0.2 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 1 | 0.2 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 1 | 0.2 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 8 | 0.2 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 8 | 0.2 |
| (1,2148) | 1:A:143:THR:H | 1:B:132:GLY:HA2 | 7 | 0.2 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD2 | 6 | 0.2 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD3 | 6 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 8 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 8 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 8 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 8 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 8 | 0.2 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 8 | 0.2 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD11 | 10 | 0.2 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD12 | 10 | 0.2 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD13 | 10 | 0.2 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG21 | 3 | 0.2 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG22 | 3 | 0.2 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG23 | 3 | 0.2 |
| (1,1796) | 1:A:152:GLN:HE21 | 1:A:149:ASP:HB2 | 2 | 0.2 |
| (1,175) | 1:A:98:SER:HA | 1:A:142:TYR:HE1 | 3 | 0.2 |
| (1,175) | 1:A:98:SER:HA | 1:A:142:TYR:HE2 | 3 | 0.2 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 6 | 0.2 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 6 | 0.2 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 6 | 0.2 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 2 | 0.2 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 2 | 0.2 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 2 | 0.2 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 2 | 0.2 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 2 | 0.2 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 2 | 0.2 |
| (1,1664) | 1:A:135:SER:H | 1:A:134:ILE:HG13 | 8 | 0.2 |
| (1,1621) | 1:A:129:ASP:H | 1:A:129:ASP:HB2 | 10 | 0.2 |
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 2 | 0.2 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD1 | 9 | 0.2 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD2 | 9 | 0.2 |
| (1,1576) | 1:A:124:HIS:H | 1:A:136:ARG:HA | 3 | 0.2 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 10 | 0.2 |
| (1,1545) | 1:A:120:ILE:H | 1:A:140:ARG:HG3 | 5 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 2 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 2 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 2 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 2 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 2 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 2 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 7 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 7 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 7 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 7 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 7 | 0.2 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 7 | 0.2 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB2 | 10 | 0.2 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB3 | 10 | 0.2 |
| (1,1489) | 1:A:114:LYS:H | 1:A:119:GLU:H | 6 | 0.2 |
| (1,1391) | 1:A:105:ALA:H | 1:A:108:GLU:HB3 | 4 | 0.2 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB2 | 6 | 0.2 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB3 | 6 | 0.2 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 2 | 0.2 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 2 | 0.2 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 2 | 0.2 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 2 | 0.2 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 2 | 0.2 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 2 | 0.2 |
| (1,1258) | 1:A:166:GLU:HG2 | 1:A:167:ALA:HA | 10 | 0.2 |
| (1,1258) | 1:A:166:GLU:HG3 | 1:A:167:ALA:HA | 10 | 0.2 |
| (1,1210) | 1:A:160:GLU:HB2 | 1:A:162:THR:HB | 1 | 0.2 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 9 | 0.2 |
| (1,1173) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB3 | 1 | 0.2 |
| (1,1173) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB3 | 1 | 0.2 |
| (1,1173) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB3 | 1 | 0.2 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 1 | 0.2 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 4 | 0.2 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD21 | 6 | 0.2 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD22 | 6 | 0.2 |
| (1,1140) | 1:A:156:SER:HB3 | 1:A:157:LEU:HD23 | 6 | 0.2 |
| (1,1128) | 1:A:155:SER:HB3 | 1:A:157:LEU:HB3 | 7 | 0.2 |
| (1,1128) | 1:A:155:SER:HB2 | 1:A:157:LEU:HB3 | 7 | 0.2 |
| (1,1077) | 1:A:153:VAL:HA | 1:A:168:PRO:HD2 | 4 | 0.2 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 9 | 0.2 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 9 | 0.2 |
| (1,102) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HB3 | 10 | 0.2 |
| (1,1014) | 1:A:148:VAL:HG11 | 1:A:170:PRO:HG3 | 7 | 0.2 |
| (1,1014) | 1:A:148:VAL:HG12 | 1:A:170:PRO:HG3 | 7 | 0.2 |
| (1,1014) | 1:A:148:VAL:HG13 | 1:A:170:PRO:HG3 | 7 | 0.2 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG11 | 5 | 0.19 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG12 | 5 | 0.19 |
| (1,987) | 1:A:148:VAL:HA | 1:A:153:VAL:HG13 | 5 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 10 | 0.19 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG3 | 9 | 0.19 |
| (1,97) | 1:A:96:ARG:HB2 | 1:A:166:GLU:HG2 | 9 | 0.19 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 9 | 0.19 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 9 | 0.19 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 9 | 0.19 |
| (1,9) | 1:A:90:HIS:HB3 | 1:A:91:THR:HA | 9 | 0.19 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 9 | 0.19 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 9 | 0.19 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 9 | 0.19 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG11 | 4 | 0.19 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG12 | 4 | 0.19 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG13 | 4 | 0.19 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG11 | 4 | 0.19 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG12 | 4 | 0.19 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG13 | 4 | 0.19 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 2 | 0.19 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 2 | 0.19 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 2 | 0.19 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 7 | 0.19 |
| (1,782) | 1:A:131:HIS:HB2 | 1:A:132:GLY:HA2 | 4 | 0.19 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD11 | 3 | 0.19 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD12 | 3 | 0.19 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD13 | 3 | 0.19 |
| (1,694) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HA | 6 | 0.19 |
| (1,694) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HA | 6 | 0.19 |
| (1,680) | 1:A:123:LYS:HA | 1:A:123:LYS:HG3 | 2 | 0.19 |
| (1,618) | 1:A:119:GLU:HG2 | 1:A:141:LYS:HG3 | 6 | 0.19 |
| (1,610) | 1:A:119:GLU:HA | 1:A:141:LYS:HD3 | 10 | 0.19 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 8 | 0.19 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 8 | 0.19 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 8 | 0.19 |
| (1,48) | 1:A:94:ARG:HD2 | 1:A:168:PRO:HA | 7 | 0.19 |
| (1,44) | 1:A:94:ARG:HG2 | 1:A:166:GLU:HB2 | 6 | 0.19 |
| (1,44) | 1:A:94:ARG:HG3 | 1:A:166:GLU:HB2 | 6 | 0.19 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD11 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD12 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG21 | 1:A:120:ILE:HD13 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD11 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD12 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG22 | 1:A:120:ILE:HD13 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD11 | 2 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD12 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG23 | 1:A:120:ILE:HD13 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD11 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD12 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG11 | 1:A:120:ILE:HD13 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD11 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD12 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG12 | 1:A:120:ILE:HD13 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD11 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD12 | 2 | 0.19 |
| (1,436) | 1:A:111:VAL:HG13 | 1:A:120:ILE:HD13 | 2 | 0.19 |
| (1,4286) | 1:B:171:LYS:H | 1:B:170:PRO:HB2 | 8 | 0.19 |
| (1,4286) | 1:B:171:LYS:H | 1:B:170:PRO:HB3 | 8 | 0.19 |
| (1,4281) | 1:B:169:MET:H | 1:B:169:MET:HG3 | 5 | 0.19 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD2 | 10 | 0.19 |
| (1,4271) | 1:B:169:MET:H | 1:B:94:ARG:HD3 | 10 | 0.19 |
| (1,4263) | 1:B:167:ALA:H | 1:B:166:GLU:HB3 | 4 | 0.19 |
| (1,419) | 1:A:111:VAL:HA | 1:A:120:ILE:HG13 | 4 | 0.19 |
| (1,419) | 1:A:111:VAL:HA | 1:A:120:ILE:HG13 | 9 | 0.19 |
| (1,4089) | 1:B:152:GLN:HE22 | 1:B:152:GLN:HB2 | 1 | 0.19 |
| (1,4089) | 1:B:152:GLN:HE22 | 1:B:152:GLN:HB2 | 2 | 0.19 |
| (1,4084) | 1:B:152:GLN:HE21 | 1:B:168:PRO:HD2 | 5 | 0.19 |
| (1,4082) | 1:B:152:GLN:HE21 | 1:B:167:ALA:HB1 | 3 | 0.19 |
| (1,4082) | 1:B:152:GLN:HE21 | 1:B:167:ALA:HB2 | 3 | 0.19 |
| (1,4082) | 1:B:152:GLN:HE21 | 1:B:167:ALA:HB3 | 3 | 0.19 |
| (1,4076) | 1:B:152:GLN:H | 1:B:170:PRO:HD2 | 1 | 0.19 |
| (1,4076) | 1:B:152:GLN:H | 1:B:170:PRO:HD3 | 1 | 0.19 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 8 | 0.19 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 8 | 0.19 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 8 | 0.19 |
| (1,395) | 1:A:110:THR:HB | 1:A:112:LYS:HG2 | 1 | 0.19 |
| (1,395) | 1:A:110:THR:HB | 1:A:112:LYS:HG3 | 1 | 0.19 |
| (1,3918) | 1:B:131:HIS:H | 1:B:130:GLU:HG2 | 1 | 0.19 |
| (1,3918) | 1:B:131:HIS:H | 1:B:130:GLU:HG3 | 1 | 0.19 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB2 | 10 | 0.19 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB3 | 10 | 0.19 |
| (1,3915) | 1:B:131:HIS:H | 1:B:129:ASP:HB3 | 8 | 0.19 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 2 | 0.19 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 2 | 0.19 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 9 | 0.19 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 9 | 0.19 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD11 | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD12 | 1 | 0.19 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD13 | 1 | 0.19 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD11 | 10 | 0.19 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD12 | 10 | 0.19 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD13 | 10 | 0.19 |
| (1,3806) | 1:B:119:GLU:H | 1:B:114:LYS:HB3 | 1 | 0.19 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 4 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 3 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 3 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 3 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 3 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 3 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 3 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 9 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 9 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 9 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 9 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 9 | 0.19 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 9 | 0.19 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 8 | 0.19 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 8 | 0.19 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 8 | 0.19 |
| (1,3726) | 1:B:111:VAL:H | 1:B:110:THR:HB | 8 | 0.19 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD21 | 8 | 0.19 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD22 | 8 | 0.19 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD23 | 8 | 0.19 |
| (1,3607) | 1:B:94:ARG:H | 1:B:168:PRO:HA | 3 | 0.19 |
| (1,3607) | 1:B:94:ARG:H | 1:B:168:PRO:HA | 4 | 0.19 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 1 | 0.19 |
| (1,3521) | 1:B:164:THR:HB | 1:B:166:GLU:HG2 | 8 | 0.19 |
| (1,3521) | 1:B:164:THR:HB | 1:B:166:GLU:HG3 | 8 | 0.19 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 8 | 0.19 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 10 | 0.19 |
| (1,3470) | 1:B:158:SER:HA | 1:B:160:GLU:HB3 | 9 | 0.19 |
| (1,3454) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB3 | 1 | 0.19 |
| (1,3454) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB3 | 1 | 0.19 |
| (1,3454) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB3 | 1 | 0.19 |
| (1,3430) | 1:B:157:LEU:HA | 1:B:163:LEU:HB3 | 4 | 0.19 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 4 | 0.19 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 5 | 0.19 |
| (1,3424) | 1:B:157:LEU:HA | 1:B:157:LEU:HB2 | 7 | 0.19 |
| (1,3391) | 1:B:155:SER:HA | 1:B:165:VAL:HA | 9 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,337) | 1:A:108:GLU:HA | 1:A:108:GLU:HG3 | 5 | 0.19 |
| (1,3358) | 1:B:153:VAL:HA | 1:B:168:PRO:HD2 | 1 | 0.19 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 4 | 0.19 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 8 | 0.19 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 8 | 0.19 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 8 | 0.19 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 8 | 0.19 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 8 | 0.19 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 8 | 0.19 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 2 | 0.19 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 2 | 0.19 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 2 | 0.19 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 2 | 0.19 |
| (1,3143) | 1:B:141:LYS:HG3 | 1:B:142:TYR:HB3 | 6 | 0.19 |
| (1,3143) | 1:B:141:LYS:HG3 | 1:B:142:TYR:HB3 | 7 | 0.19 |
| (1,3138) | 1:B:141:LYS:HG2 | 1:B:143:THR:HA | 10 | 0.19 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 7 | 0.19 |
| (1,306) | 1:A:106:PRO:HA | 1:A:106:PRO:HB3 | 8 | 0.19 |
| (1,2971) | 1:B:123:LYS:HB3 | 1:B:137:CYS:HB2 | 3 | 0.19 |
| (1,2969) | 1:B:123:LYS:HB2 | 1:B:137:CYS:HB3 | 3 | 0.19 |
| (1,2928) | 1:B:120:ILE:HG21 | 1:B:122:GLY:HA3 | 8 | 0.19 |
| (1,2928) | 1:B:120:ILE:HG22 | 1:B:122:GLY:HA3 | 8 | 0.19 |
| (1,2928) | 1:B:120:ILE:HG23 | 1:B:122:GLY:HA3 | 8 | 0.19 |
| (1,2892) | 1:B:119:GLU:HA | 1:B:141:LYS:HE2 | 10 | 0.19 |
| (1,2870) | 1:B:118:VAL:HG11 | 1:B:148:VAL:HB | 2 | 0.19 |
| (1,2870) | 1:B:118:VAL:HG12 | 1:B:148:VAL:HB | 2 | 0.19 |
| (1,2870) | 1:B:118:VAL:HG13 | 1:B:148:VAL:HB | 2 | 0.19 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG11 | 9 | 0.19 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG12 | 9 | 0.19 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG13 | 9 | 0.19 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 7 | 0.19 |
| (1,279) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA2 | 4 | 0.19 |
| (1,2755) | 1:B:112:LYS:HE3 | 1:B:114:LYS:HB3 | 9 | 0.19 |
| (1,2755) | 1:B:112:LYS:HE2 | 1:B:114:LYS:HB3 | 9 | 0.19 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD11 | 8 | 0.19 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD12 | 8 | 0.19 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD13 | 8 | 0.19 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD21 | 8 | 0.19 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD22 | 8 | 0.19 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD23 | 8 | 0.19 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 10 | 0.19 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 10 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 10 | 0.19 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 1 | 0.19 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 9 | 0.19 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 10 | 0.19 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 9 | 0.19 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 9 | 0.19 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 9 | 0.19 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 9 | 0.19 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 9 | 0.19 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 9 | 0.19 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 10 | 0.19 |
| (1,2560) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA2 | 6 | 0.19 |
| (1,2518) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HB | 4 | 0.19 |
| (1,2518) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HB | 4 | 0.19 |
| (1,2518) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HB | 4 | 0.19 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD11 | 9 | 0.19 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD12 | 9 | 0.19 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD13 | 9 | 0.19 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG3 | 7 | 0.19 |
| (1,2388) | 1:B:96:ARG:HG2 | 1:B:166:GLU:HG2 | 7 | 0.19 |
| (1,2383) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HB3 | 7 | 0.19 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG3 | 7 | 0.19 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG2 | 7 | 0.19 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 10 | 0.19 |
| (1,234) | 1:A:99:LEU:HD11 | 1:A:140:ARG:HD3 | 6 | 0.19 |
| (1,234) | 1:A:99:LEU:HD12 | 1:A:140:ARG:HD3 | 6 | 0.19 |
| (1,234) | 1:A:99:LEU:HD13 | 1:A:140:ARG:HD3 | 6 | 0.19 |
| (1,234) | 1:A:99:LEU:HD11 | 1:A:140:ARG:HD2 | 6 | 0.19 |
| (1,234) | 1:A:99:LEU:HD12 | 1:A:140:ARG:HD2 | 6 | 0.19 |
| (1,234) | 1:A:99:LEU:HD13 | 1:A:140:ARG:HD2 | 6 | 0.19 |
| (1,2329) | 1:B:94:ARG:HD2 | 1:B:168:PRO:HA | 10 | 0.19 |
| (1,2205) | 1:B:134:ILE:HD11 | 1:A:140:ARG:HD2 | 2 | 0.19 |
| (1,2205) | 1:B:134:ILE:HD12 | 1:A:140:ARG:HD2 | 2 | 0.19 |
| (1,2205) | 1:B:134:ILE:HD13 | 1:A:140:ARG:HD2 | 2 | 0.19 |
| (1,2073) | 1:B:134:ILE:HD11 | 1:A:140:ARG:HD2 | 2 | 0.19 |
| (1,2073) | 1:B:134:ILE:HD12 | 1:A:140:ARG:HD2 | 2 | 0.19 |
| (1,2073) | 1:B:134:ILE:HD13 | 1:A:140:ARG:HD2 | 2 | 0.19 |
| (1,1958) | 1:A:165:VAL:H | 1:A:166:GLU:HB3 | 5 | 0.19 |
| (1,1924) | 1:A:162:THR:H | 1:A:160:GLU:HB2 | 7 | 0.19 |
| (1,1913) | 1:A:161:GLY:H | 1:A:162:THR:HB | 2 | 0.19 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 8 | 0.19 |
| (1,1902) | 1:A:161:GLY:H | 1:A:102:ASN:HB3 | 4 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1901) | 1:A:161:GLY:H | 1:A:102:ASN:HB2 | 7 | 0.19 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD11 | 9 | 0.19 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD12 | 9 | 0.19 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD13 | 9 | 0.19 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD21 | 9 | 0.19 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD22 | 9 | 0.19 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD23 | 9 | 0.19 |
| (1,1860) | 1:A:156:SER:H | 1:A:157:LEU:HB3 | 6 | 0.19 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 4 | 0.19 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 4 | 0.19 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 4 | 0.19 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG21 | 10 | 0.19 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG22 | 10 | 0.19 |
| (1,1797) | 1:A:152:GLN:HE21 | 1:A:151:THR:HG23 | 10 | 0.19 |
| (1,1767) | 1:A:149:ASP:H | 1:A:170:PRO:HG3 | 2 | 0.19 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD2 | 1 | 0.19 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD3 | 1 | 0.19 |
| (1,1738) | 1:A:148:VAL:H | 1:A:144:LEU:HB2 | 6 | 0.19 |
| (1,17) | 1:A:93:ASP:HA | 1:A:169:MET:HG2 | 4 | 0.19 |
| (1,1647) | 1:A:132:GLY:H | 1:A:131:HIS:HB3 | 10 | 0.19 |
| (1,1634) | 1:A:131:HIS:H | 1:A:129:ASP:HB3 | 10 | 0.19 |
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 9 | 0.19 |
| (1,1608) | 1:A:128:GLN:HE22 | 1:A:128:GLN:HB2 | 3 | 0.19 |
| (1,1584) | 1:A:125:GLU:H | 1:A:126:GLU:H | 9 | 0.19 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 7 | 0.19 |
| (1,1514) | 1:A:118:VAL:H | 1:A:119:GLU:HG3 | 6 | 0.19 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 4 | 0.19 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 4 | 0.19 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 4 | 0.19 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 4 | 0.19 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 4 | 0.19 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 4 | 0.19 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD2 | 9 | 0.19 |
| (1,1478) | 1:A:114:LYS:H | 1:A:112:LYS:HD3 | 9 | 0.19 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 1 | 0.19 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 1 | 0.19 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 1 | 0.19 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 5 | 0.19 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 5 | 0.19 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 5 | 0.19 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD21 | 8 | 0.19 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD22 | 8 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD23 | 8 | 0.19 |
| (1,1383) | 1:A:102:ASN:HD22 | 1:A:161:GLY:HA3 | 4 | 0.19 |
| (1,1373) | 1:A:102:ASN:HD21 | 1:A:161:GLY:HA2 | 7 | 0.19 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD11 | 4 | 0.19 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD12 | 4 | 0.19 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD13 | 4 | 0.19 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 1 | 0.19 |
| (1,1282) | 1:A:168:PRO:HB3 | 1:A:169:MET:HA | 2 | 0.19 |
| (1,1282) | 1:A:168:PRO:HB3 | 1:A:169:MET:HA | 4 | 0.19 |
| (1,1260) | 1:A:166:GLU:HG3 | 1:A:168:PRO:HD2 | 8 | 0.19 |
| (1,1260) | 1:A:166:GLU:HG2 | 1:A:168:PRO:HD2 | 8 | 0.19 |
| (1,1260) | 1:A:166:GLU:HG2 | 1:A:168:PRO:HD3 | 8 | 0.19 |
| (1,1260) | 1:A:166:GLU:HG3 | 1:A:168:PRO:HD3 | 8 | 0.19 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 4 | 0.19 |
| (1,1173) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB3 | 3 | 0.19 |
| (1,1173) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB3 | 3 | 0.19 |
| (1,1173) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB3 | 3 | 0.19 |
| (1,1173) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB3 | 6 | 0.19 |
| (1,1173) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB3 | 6 | 0.19 |
| (1,1173) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB3 | 6 | 0.19 |
| (1,1168) | 1:A:157:LEU:HD11 | 1:A:161:GLY:HA3 | 8 | 0.19 |
| (1,1168) | 1:A:157:LEU:HD12 | 1:A:161:GLY:HA3 | 8 | 0.19 |
| (1,1168) | 1:A:157:LEU:HD13 | 1:A:161:GLY:HA3 | 8 | 0.19 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 1 | 0.19 |
| (1,1143) | 1:A:157:LEU:HA | 1:A:157:LEU:HB2 | 8 | 0.19 |
| (1,1104) | 1:A:155:SER:HA | 1:A:156:SER:HB3 | 3 | 0.19 |
| (1,1097) | 1:A:154:SER:HB3 | 1:A:155:SER:HA | 8 | 0.19 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 6 | 0.19 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG21 | 6 | 0.19 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG22 | 6 | 0.19 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG23 | 6 | 0.19 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG21 | 7 | 0.19 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG22 | 7 | 0.19 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG23 | 7 | 0.19 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 2 | 0.18 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG21 | 6 | 0.18 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG22 | 6 | 0.18 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG23 | 6 | 0.18 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG21 | 6 | 0.18 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG22 | 6 | 0.18 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG23 | 6 | 0.18 |
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG21 | 6 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG22 | 6 | 0.18 |
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG23 | 6 | 0.18 |
| (1,9) | 1:A:90:HIS:HB3 | 1:A:91:THR:HA | 8 | 0.18 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 4 | 0.18 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 4 | 0.18 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 4 | 0.18 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 10 | 0.18 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 10 | 0.18 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 10 | 0.18 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 8 | 0.18 |
| (1,849) | 1:A:141:LYS:HB2 | 1:A:141:LYS:HE2 | 6 | 0.18 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 2 | 0.18 |
| (1,749) | 1:A:128:GLN:HA | 1:A:133:TYR:HE1 | 1 | 0.18 |
| (1,749) | 1:A:128:GLN:HA | 1:A:133:TYR:HE2 | 1 | 0.18 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 5 | 0.18 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 5 | 0.18 |
| (1,664) | 1:A:121:THR:HA | 1:A:139:THR:HA | 2 | 0.18 |
| (1,664) | 1:A:121:THR:HA | 1:A:139:THR:HA | 9 | 0.18 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG21 | 7 | 0.18 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG22 | 7 | 0.18 |
| (1,6) | 1:A:90:HIS:HA | 1:A:91:THR:HG23 | 7 | 0.18 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 9 | 0.18 |
| (1,457) | 1:A:112:LYS:HB2 | 1:A:120:ILE:HA | 7 | 0.18 |
| (1,439) | 1:A:111:VAL:HG21 | 1:A:155:SER:HB2 | 8 | 0.18 |
| (1,439) | 1:A:111:VAL:HG22 | 1:A:155:SER:HB2 | 8 | 0.18 |
| (1,439) | 1:A:111:VAL:HG23 | 1:A:155:SER:HB2 | 8 | 0.18 |
| (1,439) | 1:A:111:VAL:HG11 | 1:A:155:SER:HB2 | 8 | 0.18 |
| (1,439) | 1:A:111:VAL:HG12 | 1:A:155:SER:HB2 | 8 | 0.18 |
| (1,439) | 1:A:111:VAL:HG13 | 1:A:155:SER:HB2 | 8 | 0.18 |
| (1,4270) | 1:B:169:MET:H | 1:B:94:ARG:HB2 | 6 | 0.18 |
| (1,4270) | 1:B:169:MET:H | 1:B:94:ARG:HB3 | 6 | 0.18 |
| (1,4267) | 1:B:167:ALA:H | 1:B:169:MET:H | 5 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 3 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 3 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 3 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 3 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 3 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 3 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 4 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 4 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 4 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 4 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 4 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 4 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 10 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 10 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 10 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 10 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 10 | 0.18 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 10 | 0.18 |
| (1,4196) | 1:B:162:THR:H | 1:B:102:ASN:HB2 | 4 | 0.18 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG21 | 9 | 0.18 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG22 | 9 | 0.18 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG23 | 9 | 0.18 |
| (1,4194) | 1:B:161:GLY:H | 1:B:162:THR:HB | 9 | 0.18 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 3 | 0.18 |
| (1,413) | 1:A:111:VAL:HA | 1:A:112:LYS:HG2 | 1 | 0.18 |
| (1,413) | 1:A:111:VAL:HA | 1:A:112:LYS:HG3 | 1 | 0.18 |
| (1,4125) | 1:B:154:SER:H | 1:B:168:PRO:HD2 | 7 | 0.18 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB1 | 10 | 0.18 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB2 | 10 | 0.18 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB3 | 10 | 0.18 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 8 | 0.18 |
| (1,4038) | 1:B:148:VAL:H | 1:B:170:PRO:HD2 | 9 | 0.18 |
| (1,4038) | 1:B:148:VAL:H | 1:B:170:PRO:HD3 | 9 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 4 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 4 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 4 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 5 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 5 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 5 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 6 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 6 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 6 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 10 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 10 | 0.18 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 10 | 0.18 |
| (1,3952) | 1:B:136:ARG:H | 1:B:135:SER:HB3 | 4 | 0.18 |
| (1,3936) | 1:B:134:ILE:H | 1:B:127:ARG:HG2 | 9 | 0.18 |
| (1,3903) | 1:B:129:ASP:H | 1:B:129:ASP:HB3 | 10 | 0.18 |
| (1,3894) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HA | 5 | 0.18 |
| (1,3887) | 1:B:128:GLN:H | 1:B:133:TYR:HD1 | 7 | 0.18 |
| (1,3887) | 1:B:128:GLN:H | 1:B:133:TYR:HD2 | 7 | 0.18 |
| (1,3868) | 1:B:126:GLU:H | 1:B:125:GLU:HG2 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD21 | 4 | 0.18 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD22 | 4 | 0.18 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD23 | 4 | 0.18 |
| (1,3849) | 1:B:123:LYS:H | 1:B:109:LEU:HD11 | 6 | 0.18 |
| (1,3849) | 1:B:123:LYS:H | 1:B:109:LEU:HD12 | 6 | 0.18 |
| (1,3849) | 1:B:123:LYS:H | 1:B:109:LEU:HD13 | 6 | 0.18 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 5 | 0.18 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 5 | 0.18 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 5 | 0.18 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 5 | 0.18 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 5 | 0.18 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 5 | 0.18 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD11 | 7 | 0.18 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD12 | 7 | 0.18 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD13 | 7 | 0.18 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 3 | 0.18 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 7 | 0.18 |
| (1,3748) | 1:B:113:THR:H | 1:B:112:LYS:HB2 | 6 | 0.18 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 1 | 0.18 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 1 | 0.18 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 1 | 0.18 |
| (1,3681) | 1:B:107:ASP:H | 1:B:106:PRO:HB3 | 4 | 0.18 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD11 | 1 | 0.18 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD12 | 1 | 0.18 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD13 | 1 | 0.18 |
| (1,3663) | 1:B:102:ASN:HD22 | 1:B:161:GLY:HA2 | 4 | 0.18 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD11 | 8 | 0.18 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD12 | 8 | 0.18 |
| (1,3652) | 1:B:102:ASN:HD21 | 1:B:157:LEU:HD13 | 8 | 0.18 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD11 | 10 | 0.18 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD12 | 10 | 0.18 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD13 | 10 | 0.18 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD11 | 10 | 0.18 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD12 | 10 | 0.18 |
| (1,358) | 1:A:109:LEU:HB2 | 1:A:109:LEU:HD13 | 10 | 0.18 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 3 | 0.18 |
| (1,3491) | 1:B:160:GLU:HB2 | 1:B:162:THR:HB | 3 | 0.18 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 1 | 0.18 |
| (1,349) | 1:A:109:LEU:HA | 1:A:109:LEU:HB2 | 10 | 0.18 |
| (1,346) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HG3 | 3 | 0.18 |
| (1,346) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HG2 | 3 | 0.18 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG3 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG2 | 10 | 0.18 |
| (1,337) | 1:A:108:GLU:HA | 1:A:108:GLU:HG3 | 7 | 0.18 |
| (1,3309) | 1:B:149:ASP:HA | 1:B:150:PRO:HD3 | 3 | 0.18 |
| (1,3304) | 1:B:149:ASP:HA | 1:B:149:ASP:HB3 | 3 | 0.18 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 8 | 0.18 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 8 | 0.18 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 8 | 0.18 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG11 | 4 | 0.18 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG12 | 4 | 0.18 |
| (1,3234) | 1:B:145:PRO:HB3 | 1:B:148:VAL:HG13 | 4 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 10 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 10 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 10 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 10 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 10 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 10 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 10 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 10 | 0.18 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 10 | 0.18 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 8 | 0.18 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 8 | 0.18 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 8 | 0.18 |
| (1,315) | 1:A:106:PRO:HA | 1:A:157:LEU:HB2 | 4 | 0.18 |
| (1,3112) | 1:B:139:THR:HB | 1:B:141:LYS:HE2 | 9 | 0.18 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD1 | 4 | 0.18 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD2 | 4 | 0.18 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD1 | 4 | 0.18 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD2 | 4 | 0.18 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD1 | 4 | 0.18 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD2 | 4 | 0.18 |
| (1,3060) | 1:B:131:HIS:HA | 1:B:131:HIS:HE1 | 4 | 0.18 |
| (1,3037) | 1:B:128:GLN:HB3 | 1:B:133:TYR:HD1 | 7 | 0.18 |
| (1,3037) | 1:B:128:GLN:HB3 | 1:B:133:TYR:HD2 | 7 | 0.18 |
| (1,3003) | 1:B:126:GLU:HG2 | 1:B:135:SER:HA | 7 | 0.18 |
| (1,3000) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HD1 | 2 | 0.18 |
| (1,3000) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HD2 | 2 | 0.18 |
| (1,2996) | 1:B:126:GLU:HB2 | 1:B:135:SER:HB3 | 8 | 0.18 |
| (1,2996) | 1:B:126:GLU:HB3 | 1:B:135:SER:HB3 | 8 | 0.18 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 1 | 0.18 |
| (1,296) | 1:A:105:ALA:HB1 | 1:A:107:ASP:HB2 | 7 | 0.18 |
| (1,296) | 1:A:105:ALA:HB2 | 1:A:107:ASP:HB2 | 7 | 0.18 |
| (1,296) | 1:A:105:ALA:HB3 | 1:A:107:ASP:HB2 | 7 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,296) | 1:A:105:ALA:HB1 | 1:A:107:ASP:HB2 | 9 | 0.18 |
| (1,296) | 1:A:105:ALA:HB2 | 1:A:107:ASP:HB2 | 9 | 0.18 |
| (1,296) | 1:A:105:ALA:HB3 | 1:A:107:ASP:HB2 | 9 | 0.18 |
| (1,2892) | 1:B:119:GLU:HA | 1:B:141:LYS:HE2 | 1 | 0.18 |
| (1,2891) | 1:B:119:GLU:HA | 1:B:141:LYS:HD3 | 7 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 1 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 1 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 1 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 1 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 1 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 1 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 1 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 1 | 0.18 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 1 | 0.18 |
| (1,2852) | 1:B:118:VAL:HB | 1:B:142:TYR:HD1 | 2 | 0.18 |
| (1,2852) | 1:B:118:VAL:HB | 1:B:142:TYR:HD2 | 2 | 0.18 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 5 | 0.18 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 9 | 0.18 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 9 | 0.18 |
| (1,279) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA2 | 2 | 0.18 |
| (1,2783) | 1:B:113:THR:HG21 | 1:B:150:PRO:HB3 | 9 | 0.18 |
| (1,2783) | 1:B:113:THR:HG22 | 1:B:150:PRO:HB3 | 9 | 0.18 |
| (1,2783) | 1:B:113:THR:HG23 | 1:B:150:PRO:HB3 | 9 | 0.18 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD11 | 2 | 0.18 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD12 | 2 | 0.18 |
| (1,276) | 1:A:102:ASN:HB2 | 1:A:157:LEU:HD13 | 2 | 0.18 |
| (1,2734) | 1:B:112:LYS:HA | 1:B:114:LYS:HB3 | 3 | 0.18 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD11 | 5 | 0.18 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD12 | 5 | 0.18 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD13 | 5 | 0.18 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD21 | 5 | 0.18 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD22 | 5 | 0.18 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD23 | 5 | 0.18 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 3 | 0.18 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 3 | 0.18 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 3 | 0.18 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD3 | 4 | 0.18 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD2 | 4 | 0.18 |
| (1,2619) | 1:B:108:GLU:HA | 1:B:123:LYS:HD2 | 1 | 0.18 |
| (1,2619) | 1:B:108:GLU:HA | 1:B:123:LYS:HD3 | 1 | 0.18 |
| (1,2618) | 1:B:108:GLU:HA | 1:B:108:GLU:HG3 | 2 | 0.18 |
| (1,2596) | 1:B:106:PRO:HA | 1:B:157:LEU:HB2 | 2 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2587) | 1:B:106:PRO:HA | 1:B:106:PRO:HB3 | 4 | 0.18 |
| (1,2578) | 1:B:105:ALA:HB1 | 1:B:107:ASP:HB3 | 4 | 0.18 |
| (1,2578) | 1:B:105:ALA:HB2 | 1:B:107:ASP:HB3 | 4 | 0.18 |
| (1,2578) | 1:B:105:ALA:HB3 | 1:B:107:ASP:HB3 | 4 | 0.18 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 3 | 0.18 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 3 | 0.18 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 3 | 0.18 |
| (1,2539) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HA | 9 | 0.18 |
| (1,2539) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HA | 9 | 0.18 |
| (1,2539) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HA | 9 | 0.18 |
| (1,2539) | 1:B:99:LEU:HD21 | 1:B:120:ILE:HA | 9 | 0.18 |
| (1,2539) | 1:B:99:LEU:HD22 | 1:B:120:ILE:HA | 9 | 0.18 |
| (1,2539) | 1:B:99:LEU:HD23 | 1:B:120:ILE:HA | 9 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD11 | 1:B:101:VAL:HG21 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD11 | 1:B:101:VAL:HG22 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD11 | 1:B:101:VAL:HG23 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD12 | 1:B:101:VAL:HG21 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD12 | 1:B:101:VAL:HG22 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD12 | 1:B:101:VAL:HG23 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD13 | 1:B:101:VAL:HG21 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD13 | 1:B:101:VAL:HG22 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD13 | 1:B:101:VAL:HG23 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD11 | 1:B:101:VAL:HG11 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD11 | 1:B:101:VAL:HG12 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD11 | 1:B:101:VAL:HG13 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD12 | 1:B:101:VAL:HG11 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD12 | 1:B:101:VAL:HG12 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD12 | 1:B:101:VAL:HG13 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD13 | 1:B:101:VAL:HG11 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD13 | 1:B:101:VAL:HG12 | 3 | 0.18 |
| (1,2507) | 1:B:99:LEU:HD13 | 1:B:101:VAL:HG13 | 3 | 0.18 |
| (1,2467) | 1:B:98:SER:HB2 | 1:B:164:THR:HA | 7 | 0.18 |
| (1,2442) | 1:B:97:VAL:HG21 | 1:B:166:GLU:HA | 1 | 0.18 |
| (1,2442) | 1:B:97:VAL:HG22 | 1:B:166:GLU:HA | 1 | 0.18 |
| (1,2442) | 1:B:97:VAL:HG23 | 1:B:166:GLU:HA | 1 | 0.18 |
| (1,2442) | 1:B:97:VAL:HG21 | 1:B:166:GLU:HA | 2 | 0.18 |
| (1,2442) | 1:B:97:VAL:HG22 | 1:B:166:GLU:HA | 2 | 0.18 |
| (1,2442) | 1:B:97:VAL:HG23 | 1:B:166:GLU:HA | 2 | 0.18 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG21 | 1 | 0.18 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG22 | 1 | 0.18 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG23 | 1 | 0.18 |
| (1,2398) | 1:B:96:ARG:HD2 | 1:B:166:GLU:HG2 | 6 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2398) | 1:B:96:ARG:HD3 | 1:B:166:GLU:HG3 | 6 | 0.18 |
| (1,2398) | 1:B:96:ARG:HD3 | 1:B:166:GLU:HG2 | 6 | 0.18 |
| (1,2398) | 1:B:96:ARG:HD2 | 1:B:166:GLU:HG3 | 6 | 0.18 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD3 | 6 | 0.18 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD2 | 6 | 0.18 |
| (1,237) | 1:A:99:LEU:HD21 | 1:A:101:VAL:HB | 8 | 0.18 |
| (1,237) | 1:A:99:LEU:HD22 | 1:A:101:VAL:HB | 8 | 0.18 |
| (1,237) | 1:A:99:LEU:HD23 | 1:A:101:VAL:HB | 8 | 0.18 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG21 | 9 | 0.18 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG22 | 9 | 0.18 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG23 | 9 | 0.18 |
| (1,2332) | 1:B:95:TRP:HA | 1:B:95:TRP:HB2 | 7 | 0.18 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 6 | 0.18 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD3 | 1 | 0.18 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD2 | 1 | 0.18 |
| (1,2310) | 1:B:94:ARG:HA | 1:B:168:PRO:HA | 5 | 0.18 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG21 | 9 | 0.18 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG22 | 9 | 0.18 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG23 | 9 | 0.18 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG21 | 9 | 0.18 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG22 | 9 | 0.18 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG23 | 9 | 0.18 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD2 | 4 | 0.18 |
| (1,1990) | 1:A:169:MET:H | 1:A:94:ARG:HD3 | 4 | 0.18 |
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 8 | 0.18 |
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 9 | 0.18 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 5 | 0.18 |
| (1,1920) | 1:A:162:THR:H | 1:A:158:SER:HB2 | 2 | 0.18 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 4 | 0.18 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB1 | 3 | 0.18 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB2 | 3 | 0.18 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB3 | 3 | 0.18 |
| (1,1745) | 1:A:148:VAL:H | 1:A:146:PRO:HD2 | 10 | 0.18 |
| (1,1745) | 1:A:148:VAL:H | 1:A:146:PRO:HD3 | 10 | 0.18 |
| (1,1655) | 1:A:134:ILE:H | 1:A:127:ARG:HG2 | 6 | 0.18 |
| (1,1655) | 1:A:134:ILE:H | 1:A:127:ARG:HG2 | 10 | 0.18 |
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 5 | 0.18 |
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 10 | 0.18 |
| (1,1597) | 1:A:128:GLN:H | 1:A:127:ARG:HB3 | 7 | 0.18 |
| (1,1591) | 1:A:126:GLU:H | 1:A:135:SER:HB2 | 4 | 0.18 |
| (1,1591) | 1:A:126:GLU:H | 1:A:135:SER:HB3 | 4 | 0.18 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 1 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 6 | 0.18 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 8 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG21 | 6 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG22 | 6 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG23 | 6 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG11 | 6 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG12 | 6 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG13 | 6 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG21 | 7 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG22 | 7 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG23 | 7 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG11 | 7 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG12 | 7 | 0.18 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG13 | 7 | 0.18 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 6 | 0.18 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 5 | 0.18 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 5 | 0.18 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 5 | 0.18 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 5 | 0.18 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 5 | 0.18 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 5 | 0.18 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB2 | 1 | 0.18 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB3 | 1 | 0.18 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 10 | 0.18 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 10 | 0.18 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 10 | 0.18 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD21 | 10 | 0.18 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD22 | 10 | 0.18 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD23 | 10 | 0.18 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD21 | 10 | 0.18 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD22 | 10 | 0.18 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD23 | 10 | 0.18 |
| (1,1391) | 1:A:105:ALA:H | 1:A:108:GLU:HB3 | 1 | 0.18 |
| (1,1391) | 1:A:105:ALA:H | 1:A:108:GLU:HB3 | 7 | 0.18 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD11 | 1 | 0.18 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD12 | 1 | 0.18 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD13 | 1 | 0.18 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD11 | 5 | 0.18 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD12 | 5 | 0.18 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD13 | 5 | 0.18 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG11 | 8 | 0.18 |
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG12 | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,129) | 1:A:97:VAL:HB | 1:A:148:VAL:HG13 | 8 | 0.18 |
| (1,1276) | 1:A:168:PRO:HA | 1:A:169:MET:HG2 | 6 | 0.18 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG2 | 10 | 0.18 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG3 | 10 | 0.18 |
| (1,1206) | 1:A:159:PRO:HD2 | 1:A:160:GLU:HB3 | 7 | 0.18 |
| (1,1168) | 1:A:157:LEU:HD11 | 1:A:161:GLY:HA3 | 5 | 0.18 |
| (1,1168) | 1:A:157:LEU:HD12 | 1:A:161:GLY:HA3 | 5 | 0.18 |
| (1,1168) | 1:A:157:LEU:HD13 | 1:A:161:GLY:HA3 | 5 | 0.18 |
| (1,1128) | 1:A:155:SER:HB3 | 1:A:157:LEU:HB3 | 9 | 0.18 |
| (1,1128) | 1:A:155:SER:HB2 | 1:A:157:LEU:HB3 | 9 | 0.18 |
| (1,1065) | 1:A:152:GLN:HB2 | 1:A:169:MET:HA | 6 | 0.18 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 2 | 0.18 |
| (1,1014) | 1:A:148:VAL:HG11 | 1:A:170:PRO:HG3 | 6 | 0.18 |
| (1,1014) | 1:A:148:VAL:HG12 | 1:A:170:PRO:HG3 | 6 | 0.18 |
| (1,1014) | 1:A:148:VAL:HG13 | 1:A:170:PRO:HG3 | 6 | 0.18 |
| (1,992) | 1:A:148:VAL:HA | 1:A:170:PRO:HB3 | 7 | 0.17 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 7 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 1 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 1 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 1 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 3 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 3 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 3 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 6 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 6 | 0.17 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 6 | 0.17 |
| (1,858) | 1:A:141:LYS:HG3 | 1:A:141:LYS:HE2 | 4 | 0.17 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 7 | 0.17 |
| (1,747) | 1:A:128:GLN:HA | 1:A:133:TYR:HB2 | 10 | 0.17 |
| (1,726) | 1:A:126:GLU:HG3 | 1:A:127:ARG:HG2 | 7 | 0.17 |
| (1,680) | 1:A:123:LYS:HA | 1:A:123:LYS:HG3 | 4 | 0.17 |
| (1,611) | 1:A:119:GLU:HA | 1:A:141:LYS:HE2 | 5 | 0.17 |
| (1,605) | 1:A:119:GLU:HA | 1:A:120:ILE:HG13 | 8 | 0.17 |
| (1,602) | 1:A:119:GLU:HA | 1:A:119:GLU:HG3 | 5 | 0.17 |
| (1,602) | 1:A:119:GLU:HA | 1:A:119:GLU:HG3 | 6 | 0.17 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 3 | 0.17 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 3 | 0.17 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 3 | 0.17 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG11 | 1 | 0.17 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG12 | 1 | 0.17 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG13 | 1 | 0.17 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG21 | 1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG22 | 1 | 0.17 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG23 | 1 | 0.17 |
| (1,478) | 1:A:112:LYS:HE2 | 1:A:121:THR:HB | 9 | 0.17 |
| (1,478) | 1:A:112:LYS:HE3 | 1:A:121:THR:HB | 9 | 0.17 |
| (1,465) | 1:A:112:LYS:HG2 | 1:A:118:VAL:HA | 4 | 0.17 |
| (1,465) | 1:A:112:LYS:HG3 | 1:A:118:VAL:HA | 4 | 0.17 |
| (1,439) | 1:A:111:VAL:HG21 | 1:A:155:SER:HB2 | 3 | 0.17 |
| (1,439) | 1:A:111:VAL:HG22 | 1:A:155:SER:HB2 | 3 | 0.17 |
| (1,439) | 1:A:111:VAL:HG23 | 1:A:155:SER:HB2 | 3 | 0.17 |
| (1,439) | 1:A:111:VAL:HG11 | 1:A:155:SER:HB2 | 3 | 0.17 |
| (1,439) | 1:A:111:VAL:HG12 | 1:A:155:SER:HB2 | 3 | 0.17 |
| (1,439) | 1:A:111:VAL:HG13 | 1:A:155:SER:HB2 | 3 | 0.17 |
| (1,439) | 1:A:111:VAL:HG21 | 1:A:155:SER:HB2 | 5 | 0.17 |
| (1,439) | 1:A:111:VAL:HG22 | 1:A:155:SER:HB2 | 5 | 0.17 |
| (1,439) | 1:A:111:VAL:HG23 | 1:A:155:SER:HB2 | 5 | 0.17 |
| (1,439) | 1:A:111:VAL:HG11 | 1:A:155:SER:HB2 | 5 | 0.17 |
| (1,439) | 1:A:111:VAL:HG12 | 1:A:155:SER:HB2 | 5 | 0.17 |
| (1,439) | 1:A:111:VAL:HG13 | 1:A:155:SER:HB2 | 5 | 0.17 |
| (1,4197) | 1:B:162:THR:H | 1:B:102:ASN:HB3 | 3 | 0.17 |
| (1,4194) | 1:B:161:GLY:H | 1:B:162:THR:HB | 1 | 0.17 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 4 | 0.17 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 10 | 0.17 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 3 | 0.17 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 3 | 0.17 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 3 | 0.17 |
| (1,3910) | 1:B:129:ASP:H | 1:B:133:TYR:HB2 | 6 | 0.17 |
| (1,3904) | 1:B:129:ASP:H | 1:B:130:GLU:HG2 | 3 | 0.17 |
| (1,3904) | 1:B:129:ASP:H | 1:B:130:GLU:HG3 | 3 | 0.17 |
| (1,3894) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HA | 2 | 0.17 |
| (1,3878) | 1:B:128:GLN:H | 1:B:127:ARG:HB3 | 9 | 0.17 |
| (1,3869) | 1:B:126:GLU:H | 1:B:125:GLU:HG3 | 7 | 0.17 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB1 | 9 | 0.17 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB2 | 9 | 0.17 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB3 | 9 | 0.17 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 6 | 0.17 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 3 | 0.17 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 8 | 0.17 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 8 | 0.17 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 8 | 0.17 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 8 | 0.17 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 8 | 0.17 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 8 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD2 | 6 | 0.17 |
| (1,3759) | 1:B:114:LYS:H | 1:B:112:LYS:HD3 | 6 | 0.17 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB2 | 9 | 0.17 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB3 | 9 | 0.17 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG21 | 5 | 0.17 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG22 | 5 | 0.17 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG23 | 5 | 0.17 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG11 | 5 | 0.17 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG12 | 5 | 0.17 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG13 | 5 | 0.17 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 7 | 0.17 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 7 | 0.17 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 7 | 0.17 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 10 | 0.17 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 10 | 0.17 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 10 | 0.17 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 10 | 0.17 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 10 | 0.17 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 10 | 0.17 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 10 | 0.17 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 10 | 0.17 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 10 | 0.17 |
| (1,37) | 1:A:94:ARG:HB2 | 1:A:96:ARG:HA | 5 | 0.17 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 1 | 0.17 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 1 | 0.17 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 1 | 0.17 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 1 | 0.17 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 1 | 0.17 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 1 | 0.17 |
| (1,3663) | 1:B:102:ASN:HD22 | 1:B:161:GLY:HA2 | 7 | 0.17 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD21 | 2 | 0.17 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD22 | 2 | 0.17 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD23 | 2 | 0.17 |
| (1,3605) | 1:B:94:ARG:H | 1:B:94:ARG:HG2 | 9 | 0.17 |
| (1,3605) | 1:B:94:ARG:H | 1:B:94:ARG:HG3 | 9 | 0.17 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 7 | 0.17 |
| (1,3569) | 1:B:169:MET:HA | 1:B:169:MET:HG2 | 7 | 0.17 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD3 | 8 | 0.17 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD2 | 8 | 0.17 |
| (1,3460) | 1:B:157:LEU:HD21 | 1:B:163:LEU:HB3 | 10 | 0.17 |
| (1,3460) | 1:B:157:LEU:HD22 | 1:B:163:LEU:HB3 | 10 | 0.17 |
| (1,3460) | 1:B:157:LEU:HD23 | 1:B:163:LEU:HB3 | 10 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3455) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HG | 5 | 0.17 |
| (1,3455) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HG | 5 | 0.17 |
| (1,3455) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HG | 5 | 0.17 |
| (1,3454) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB3 | 2 | 0.17 |
| (1,3454) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB3 | 2 | 0.17 |
| (1,3454) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB3 | 2 | 0.17 |
| (1,3454) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB3 | 10 | 0.17 |
| (1,3454) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB3 | 10 | 0.17 |
| (1,3454) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB3 | 10 | 0.17 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 6 | 0.17 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 6 | 0.17 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 6 | 0.17 |
| (1,3391) | 1:B:155:SER:HA | 1:B:165:VAL:HA | 1 | 0.17 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG3 | 8 | 0.17 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG2 | 8 | 0.17 |
| (1,3358) | 1:B:153:VAL:HA | 1:B:168:PRO:HD2 | 9 | 0.17 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 4 | 0.17 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 4 | 0.17 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 4 | 0.17 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 4 | 0.17 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 8 | 0.17 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 10 | 0.17 |
| (1,331) | 1:A:107:ASP:HA | 1:A:108:GLU:HG2 | 6 | 0.17 |
| (1,3302) | 1:B:148:VAL:HG21 | 1:B:169:MET:HB3 | 2 | 0.17 |
| (1,3302) | 1:B:148:VAL:HG22 | 1:B:169:MET:HB3 | 2 | 0.17 |
| (1,3302) | 1:B:148:VAL:HG23 | 1:B:169:MET:HB3 | 2 | 0.17 |
| (1,3295) | 1:B:148:VAL:HG11 | 1:B:170:PRO:HG3 | 6 | 0.17 |
| (1,3295) | 1:B:148:VAL:HG12 | 1:B:170:PRO:HG3 | 6 | 0.17 |
| (1,3295) | 1:B:148:VAL:HG13 | 1:B:170:PRO:HG3 | 6 | 0.17 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD21 | 2 | 0.17 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD22 | 2 | 0.17 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:109:LEU:HD23 | 2 | 0.17 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD21 | 2 | 0.17 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD22 | 2 | 0.17 |
| (1,328) | 1:A:106:PRO:HD2 | 1:A:157:LEU:HD23 | 2 | 0.17 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 2 | 0.17 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 2 | 0.17 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 2 | 0.17 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG11 | 4 | 0.17 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG12 | 4 | 0.17 |
| (1,3268) | 1:B:148:VAL:HA | 1:B:153:VAL:HG13 | 4 | 0.17 |
| (1,3249) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA3 | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 6 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 7 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG21 | 8 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG22 | 8 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD21 | 1:B:148:VAL:HG23 | 8 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG21 | 8 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG22 | 8 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD22 | 1:B:148:VAL:HG23 | 8 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG21 | 8 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG22 | 8 | 0.17 |
| (1,3219) | 1:B:144:LEU:HD23 | 1:B:148:VAL:HG23 | 8 | 0.17 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 1 | 0.17 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 1 | 0.17 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 1 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 2 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 2 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 2 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 9 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 9 | 0.17 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 9 | 0.17 |
| (1,3138) | 1:B:141:LYS:HG2 | 1:B:143:THR:HA | 8 | 0.17 |
| (1,3133) | 1:B:141:LYS:HG2 | 1:B:141:LYS:HE2 | 7 | 0.17 |
| (1,3130) | 1:B:141:LYS:HB2 | 1:B:141:LYS:HE2 | 9 | 0.17 |
| (1,3087) | 1:B:134:ILE:HG21 | 1:B:135:SER:HB3 | 10 | 0.17 |
| (1,3087) | 1:B:134:ILE:HG22 | 1:B:135:SER:HB3 | 10 | 0.17 |
| (1,3087) | 1:B:134:ILE:HG23 | 1:B:135:SER:HB3 | 10 | 0.17 |
| (1,3087) | 1:B:134:ILE:HD11 | 1:B:135:SER:HB3 | 10 | 0.17 |
| (1,3087) | 1:B:134:ILE:HD12 | 1:B:135:SER:HB3 | 10 | 0.17 |
| (1,3087) | 1:B:134:ILE:HD13 | 1:B:135:SER:HB3 | 10 | 0.17 |
| (1,3027) | 1:B:128:GLN:HA | 1:B:128:GLN:HG3 | 8 | 0.17 |
| (1,3014) | 1:B:126:GLU:HG3 | 1:B:135:SER:HB3 | 2 | 0.17 |
| (1,3000) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HD1 | 3 | 0.17 |
| (1,3000) | 1:B:126:GLU:HG2 | 1:B:133:TYR:HD2 | 3 | 0.17 |
| (1,2994) | 1:B:126:GLU:HB2 | 1:B:133:TYR:HB3 | 1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2994) | 1:B:126:GLU:HB3 | 1:B:133:TYR:HB3 | 1 | 0.17 |
| (1,2945) | 1:B:121:THR:HA | 1:B:139:THR:HA | 8 | 0.17 |
| (1,29) | 1:A:94:ARG:HA | 1:A:168:PRO:HA | 6 | 0.17 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 4 | 0.17 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 4 | 0.17 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 4 | 0.17 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 6 | 0.17 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 6 | 0.17 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 6 | 0.17 |
| (1,2831) | 1:B:117:VAL:HA | 1:B:148:VAL:HB | 8 | 0.17 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG21 | 4 | 0.17 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG22 | 4 | 0.17 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG23 | 4 | 0.17 |
| (1,2790) | 1:B:114:LYS:HA | 1:B:114:LYS:HB2 | 1 | 0.17 |
| (1,279) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA2 | 6 | 0.17 |
| (1,2757) | 1:B:112:LYS:HE2 | 1:B:119:GLU:HG3 | 6 | 0.17 |
| (1,2757) | 1:B:112:LYS:HE3 | 1:B:119:GLU:HG3 | 6 | 0.17 |
| (1,2700) | 1:B:111:VAL:HA | 1:B:120:ILE:HG13 | 2 | 0.17 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 7 | 0.17 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 5 | 0.17 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 5 | 0.17 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 5 | 0.17 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 5 | 0.17 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 5 | 0.17 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 5 | 0.17 |
| (1,2664) | 1:B:109:LEU:HD21 | 1:B:122:GLY:HA3 | 1 | 0.17 |
| (1,2664) | 1:B:109:LEU:HD22 | 1:B:122:GLY:HA3 | 1 | 0.17 |
| (1,2664) | 1:B:109:LEU:HD23 | 1:B:122:GLY:HA3 | 1 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 5 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 5 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 5 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 5 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 5 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 5 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 5 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 5 | 0.17 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 5 | 0.17 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD3 | 8 | 0.17 |
| (1,2628) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HD2 | 8 | 0.17 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 7 | 0.17 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 7 | 0.17 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2561) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA3 | 6 | 0.17 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD11 | 7 | 0.17 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD12 | 7 | 0.17 |
| (1,2550) | 1:B:101:VAL:HB | 1:B:157:LEU:HD13 | 7 | 0.17 |
| (1,2546) | 1:B:100:ASP:HB3 | 1:B:162:THR:HA | 2 | 0.17 |
| (1,2518) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HB | 3 | 0.17 |
| (1,2518) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HB | 3 | 0.17 |
| (1,2518) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HB | 3 | 0.17 |
| (1,2518) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HB | 5 | 0.17 |
| (1,2518) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HB | 5 | 0.17 |
| (1,2518) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HB | 5 | 0.17 |
| (1,2301) | 1:B:93:ASP:HB3 | 1:B:94:ARG:HA | 4 | 0.17 |
| (1,23) | 1:A:94:ARG:HA | 1:A:94:ARG:HB3 | 8 | 0.17 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG21 | 7 | 0.17 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG22 | 7 | 0.17 |
| (1,2289) | 1:B:90:HIS:HB2 | 1:B:91:THR:HG23 | 7 | 0.17 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 8 | 0.17 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 8 | 0.17 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 8 | 0.17 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 8 | 0.17 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 10 | 0.17 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 10 | 0.17 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 10 | 0.17 |
| (1,2152) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2152) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2152) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2152) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2152) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2152) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 8 | 0.17 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 8 | 0.17 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 8 | 0.17 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 8 | 0.17 |
| (1,2020) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2020) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2020) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2020) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2020) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,2020) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 8 | 0.17 |
| (1,1998) | 1:A:169:MET:H | 1:A:169:MET:HB2 | 6 | 0.17 |
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 7 | 0.17 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG21 | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG22 | 3 | 0.17 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG23 | 3 | 0.17 |
| (1,1901) | 1:A:161:GLY:H | 1:A:102:ASN:HB2 | 9 | 0.17 |
| (1,1799) | 1:A:152:GLN:HE21 | 1:A:152:GLN:HB3 | 5 | 0.17 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD2 | 9 | 0.17 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD3 | 9 | 0.17 |
| (1,1756) | 1:A:148:VAL:H | 1:A:170:PRO:HG3 | 6 | 0.17 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 8 | 0.17 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 8 | 0.17 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 8 | 0.17 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 8 | 0.17 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 8 | 0.17 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 8 | 0.17 |
| (1,1634) | 1:A:131:HIS:H | 1:A:129:ASP:HB3 | 5 | 0.17 |
| (1,1634) | 1:A:131:HIS:H | 1:A:129:ASP:HB3 | 6 | 0.17 |
| (1,1588) | 1:A:126:GLU:H | 1:A:125:GLU:HG3 | 6 | 0.17 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG21 | 9 | 0.17 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG22 | 9 | 0.17 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG23 | 9 | 0.17 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG11 | 9 | 0.17 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG12 | 9 | 0.17 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG13 | 9 | 0.17 |
| (1,1525) | 1:A:119:GLU:H | 1:A:114:LYS:HB3 | 6 | 0.17 |
| (1,1525) | 1:A:119:GLU:H | 1:A:114:LYS:HB3 | 9 | 0.17 |
| (1,1489) | 1:A:114:LYS:H | 1:A:119:GLU:H | 3 | 0.17 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 5 | 0.17 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 2 | 0.17 |
| (1,1391) | 1:A:105:ALA:H | 1:A:108:GLU:HB3 | 6 | 0.17 |
| (1,1389) | 1:A:105:ALA:H | 1:A:106:PRO:HD3 | 3 | 0.17 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD21 | 10 | 0.17 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD22 | 10 | 0.17 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD23 | 10 | 0.17 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD11 | 1 | 0.17 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD12 | 1 | 0.17 |
| (1,1380) | 1:A:102:ASN:HD22 | 1:A:157:LEU:HD13 | 1 | 0.17 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 2 | 0.17 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 5 | 0.17 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 3 | 0.17 |
| (1,1168) | 1:A:157:LEU:HD11 | 1:A:161:GLY:HA3 | 9 | 0.17 |
| (1,1168) | 1:A:157:LEU:HD12 | 1:A:161:GLY:HA3 | 9 | 0.17 |
| (1,1168) | 1:A:157:LEU:HD13 | 1:A:161:GLY:HA3 | 9 | 0.17 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 1 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD11 | 6 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD12 | 6 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD13 | 6 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD21 | 6 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD22 | 6 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD23 | 6 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD11 | 7 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD12 | 7 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD13 | 7 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD21 | 7 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD22 | 7 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD23 | 7 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD11 | 8 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD12 | 8 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD13 | 8 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD21 | 8 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD22 | 8 | 0.17 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD23 | 8 | 0.17 |
| (1,1104) | 1:A:155:SER:HA | 1:A:156:SER:HB3 | 6 | 0.17 |
| (1,1064) | 1:A:152:GLN:HB2 | 1:A:168:PRO:HD3 | 4 | 0.17 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG21 | 7 | 0.17 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG22 | 7 | 0.17 |
| (1,1046) | 1:A:150:PRO:HD2 | 1:A:151:THR:HG23 | 7 | 0.17 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 1 | 0.17 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 5 | 0.17 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 4 | 0.17 |
| (1,101) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HA | 8 | 0.17 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 3 | 0.16 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 8 | 0.16 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 9 | 0.16 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 1 | 0.16 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 1 | 0.16 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 1 | 0.16 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD11 | 8 | 0.16 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD12 | 8 | 0.16 |
| (1,896) | 1:A:143:THR:HB | 1:A:144:LEU:HD13 | 8 | 0.16 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 4 | 0.16 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 4 | 0.16 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 4 | 0.16 |
| (1,858) | 1:A:141:LYS:HG3 | 1:A:141:LYS:HE2 | 3 | 0.16 |
| (1,856) | 1:A:141:LYS:HG2 | 1:A:142:TYR:HB3 | 3 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,831) | 1:A:139:THR:HB | 1:A:141:LYS:HE2 | 3 | 0.16 |
| (1,779) | 1:A:131:HIS:HA | 1:A:131:HIS:HE1 | 2 | 0.16 |
| (1,773) | 1:A:130:GLU:HA | 1:A:130:GLU:HG3 | 2 | 0.16 |
| (1,764) | 1:A:129:ASP:HA | 1:A:129:ASP:HB3 | 2 | 0.16 |
| (1,756) | 1:A:128:GLN:HB3 | 1:A:133:TYR:HD1 | 8 | 0.16 |
| (1,756) | 1:A:128:GLN:HB3 | 1:A:133:TYR:HD2 | 8 | 0.16 |
| (1,723) | 1:A:126:GLU:HG2 | 1:A:135:SER:HB2 | 6 | 0.16 |
| (1,703) | 1:A:125:GLU:HA | 1:A:135:SER:HB2 | 5 | 0.16 |
| (1,695) | 1:A:123:LYS:HD2 | 1:A:137:CYS:HB2 | 7 | 0.16 |
| (1,695) | 1:A:123:LYS:HD3 | 1:A:137:CYS:HB2 | 7 | 0.16 |
| (1,680) | 1:A:123:LYS:HA | 1:A:123:LYS:HG3 | 9 | 0.16 |
| (1,680) | 1:A:123:LYS:HA | 1:A:123:LYS:HG3 | 10 | 0.16 |
| (1,654) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HD2 | 10 | 0.16 |
| (1,654) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HD2 | 10 | 0.16 |
| (1,654) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HD2 | 10 | 0.16 |
| (1,648) | 1:A:120:ILE:HG21 | 1:A:139:THR:HA | 10 | 0.16 |
| (1,648) | 1:A:120:ILE:HG22 | 1:A:139:THR:HA | 10 | 0.16 |
| (1,648) | 1:A:120:ILE:HG23 | 1:A:139:THR:HA | 10 | 0.16 |
| (1,605) | 1:A:119:GLU:HA | 1:A:120:ILE:HG13 | 1 | 0.16 |
| (1,605) | 1:A:119:GLU:HA | 1:A:120:ILE:HG13 | 10 | 0.16 |
| (1,60) | 1:A:95:TRP:HB2 | 1:A:95:TRP:HE3 | 3 | 0.16 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 7 | 0.16 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 7 | 0.16 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 7 | 0.16 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 9 | 0.16 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 9 | 0.16 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 9 | 0.16 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG21 | 4 | 0.16 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG22 | 4 | 0.16 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG23 | 4 | 0.16 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG21 | 6 | 0.16 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG22 | 6 | 0.16 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG23 | 6 | 0.16 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 2 | 0.16 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 2 | 0.16 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 2 | 0.16 |
| (1,502) | 1:A:113:THR:HG21 | 1:A:150:PRO:HB3 | 1 | 0.16 |
| (1,502) | 1:A:113:THR:HG22 | 1:A:150:PRO:HB3 | 1 | 0.16 |
| (1,502) | 1:A:113:THR:HG23 | 1:A:150:PRO:HB3 | 1 | 0.16 |
| (1,502) | 1:A:113:THR:HG21 | 1:A:150:PRO:HB3 | 8 | 0.16 |
| (1,502) | 1:A:113:THR:HG22 | 1:A:150:PRO:HB3 | 8 | 0.16 |
| (1,502) | 1:A:113:THR:HG23 | 1:A:150:PRO:HB3 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4278) | 1:B:169:MET:H | 1:B:169:MET:HA | 5 | 0.16 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG2 | 2 | 0.16 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG3 | 2 | 0.16 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD11 | 9 | 0.16 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD12 | 9 | 0.16 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD13 | 9 | 0.16 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD21 | 9 | 0.16 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD22 | 9 | 0.16 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD23 | 9 | 0.16 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 6 | 0.16 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 6 | 0.16 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 6 | 0.16 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 6 | 0.16 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 6 | 0.16 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 6 | 0.16 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG21 | 5 | 0.16 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG22 | 5 | 0.16 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG23 | 5 | 0.16 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG21 | 10 | 0.16 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG22 | 10 | 0.16 |
| (1,4195) | 1:B:161:GLY:H | 1:B:162:THR:HG23 | 10 | 0.16 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 8 | 0.16 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 9 | 0.16 |
| (1,4182) | 1:B:161:GLY:H | 1:B:102:ASN:HB2 | 1 | 0.16 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG21 | 9 | 0.16 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG22 | 9 | 0.16 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG23 | 9 | 0.16 |
| (1,4125) | 1:B:154:SER:H | 1:B:168:PRO:HD2 | 3 | 0.16 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 10 | 0.16 |
| (1,4036) | 1:B:148:VAL:H | 1:B:170:PRO:HB2 | 3 | 0.16 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG21 | 9 | 0.16 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG22 | 9 | 0.16 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG23 | 9 | 0.16 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG11 | 9 | 0.16 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG12 | 9 | 0.16 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG13 | 9 | 0.16 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB2 | 1 | 0.16 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB3 | 1 | 0.16 |
| (1,3907) | 1:B:129:ASP:H | 1:B:132:GLY:HA3 | 2 | 0.16 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD21 | 10 | 0.16 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD22 | 10 | 0.16 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD23 | 10 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB1 | 5 | 0.16 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB2 | 5 | 0.16 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB3 | 5 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 4 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 4 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 4 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 4 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 4 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 4 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 6 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 6 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 6 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 6 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 6 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 6 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 9 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 9 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 9 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 9 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 9 | 0.16 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 9 | 0.16 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD11 | 2 | 0.16 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD12 | 2 | 0.16 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD13 | 2 | 0.16 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD11 | 9 | 0.16 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD12 | 9 | 0.16 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD13 | 9 | 0.16 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 2 | 0.16 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 2 | 0.16 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 2 | 0.16 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 2 | 0.16 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 2 | 0.16 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 2 | 0.16 |
| (1,3770) | 1:B:114:LYS:H | 1:B:119:GLU:H | 3 | 0.16 |
| (1,3770) | 1:B:114:LYS:H | 1:B:119:GLU:H | 10 | 0.16 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 4 | 0.16 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 4 | 0.16 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 4 | 0.16 |
| (1,3699) | 1:B:108:GLU:H | 1:B:108:GLU:HG2 | 2 | 0.16 |
| (1,3699) | 1:B:108:GLU:H | 1:B:108:GLU:HG3 | 2 | 0.16 |
| (1,3699) | 1:B:108:GLU:H | 1:B:108:GLU:HG2 | 3 | 0.16 |
| (1,3699) | 1:B:108:GLU:H | 1:B:108:GLU:HG3 | 3 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 4 | 0.16 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 4 | 0.16 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 4 | 0.16 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 4 | 0.16 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 4 | 0.16 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 4 | 0.16 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD21 | 6 | 0.16 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD22 | 6 | 0.16 |
| (1,3662) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD23 | 6 | 0.16 |
| (1,3641) | 1:B:101:VAL:H | 1:B:100:ASP:HB2 | 6 | 0.16 |
| (1,3641) | 1:B:101:VAL:H | 1:B:100:ASP:HB3 | 6 | 0.16 |
| (1,3569) | 1:B:169:MET:HA | 1:B:169:MET:HG2 | 2 | 0.16 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 4 | 0.16 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD2 | 2 | 0.16 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD2 | 2 | 0.16 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD3 | 2 | 0.16 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD3 | 2 | 0.16 |
| (1,3521) | 1:B:164:THR:HB | 1:B:166:GLU:HG2 | 5 | 0.16 |
| (1,3521) | 1:B:164:THR:HB | 1:B:166:GLU:HG3 | 5 | 0.16 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 2 | 0.16 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 2 | 0.16 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 2 | 0.16 |
| (1,3430) | 1:B:157:LEU:HA | 1:B:163:LEU:HB3 | 5 | 0.16 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG3 | 4 | 0.16 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG2 | 4 | 0.16 |
| (1,337) | 1:A:108:GLU:HA | 1:A:108:GLU:HG3 | 1 | 0.16 |
| (1,3360) | 1:B:153:VAL:HB | 1:B:154:SER:HA | 9 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG21 | 7 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG22 | 7 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG23 | 7 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG21 | 8 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG22 | 8 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG23 | 8 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG21 | 10 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG22 | 10 | 0.16 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG23 | 10 | 0.16 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 2 | 0.16 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 6 | 0.16 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 9 | 0.16 |
| (1,331) | 1:A:107:ASP:HA | 1:A:108:GLU:HG2 | 1 | 0.16 |
| (1,3292) | 1:B:148:VAL:HG11 | 1:B:169:MET:HA | 1 | 0.16 |
| (1,3292) | 1:B:148:VAL:HG12 | 1:B:169:MET:HA | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3292) | 1:B:148:VAL:HG13 | 1:B:169:MET:HA | 1 | 0.16 |
| (1,3292) | 1:B:148:VAL:HG11 | 1:B:169:MET:HA | 2 | 0.16 |
| (1,3292) | 1:B:148:VAL:HG12 | 1:B:169:MET:HA | 2 | 0.16 |
| (1,3292) | 1:B:148:VAL:HG13 | 1:B:169:MET:HA | 2 | 0.16 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 4 | 0.16 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD3 | 8 | 0.16 |
| (1,3197) | 1:B:144:LEU:HB3 | 1:B:146:PRO:HD2 | 8 | 0.16 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 5 | 0.16 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 5 | 0.16 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 5 | 0.16 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 5 | 0.16 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 6 | 0.16 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 2 | 0.16 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 8 | 0.16 |
| (1,3005) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB3 | 9 | 0.16 |
| (1,2980) | 1:B:125:GLU:HA | 1:B:125:GLU:HG2 | 2 | 0.16 |
| (1,298) | 1:A:105:ALA:HB1 | 1:A:108:GLU:HB2 | 1 | 0.16 |
| (1,298) | 1:A:105:ALA:HB2 | 1:A:108:GLU:HB2 | 1 | 0.16 |
| (1,298) | 1:A:105:ALA:HB3 | 1:A:108:GLU:HB2 | 1 | 0.16 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 8 | 0.16 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 9 | 0.16 |
| (1,2928) | 1:B:120:ILE:HG21 | 1:B:122:GLY:HA3 | 4 | 0.16 |
| (1,2928) | 1:B:120:ILE:HG22 | 1:B:122:GLY:HA3 | 4 | 0.16 |
| (1,2928) | 1:B:120:ILE:HG23 | 1:B:122:GLY:HA3 | 4 | 0.16 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 6 | 0.16 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 6 | 0.16 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 6 | 0.16 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 8 | 0.16 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 8 | 0.16 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 8 | 0.16 |
| (1,2886) | 1:B:119:GLU:HA | 1:B:120:ILE:HG13 | 9 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 3 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 3 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 3 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 3 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 3 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 3 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 3 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 3 | 0.16 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 3 | 0.16 |
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD21 | 4 | 0.16 |
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD22 | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD23 | 4 | 0.16 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 9 | 0.16 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 9 | 0.16 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 9 | 0.16 |
| (1,2831) | 1:B:117:VAL:HA | 1:B:148:VAL:HB | 3 | 0.16 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 4 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 2 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 2 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 2 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 2 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 2 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 2 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 9 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 9 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 9 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 9 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 9 | 0.16 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 9 | 0.16 |
| (1,2715) | 1:B:111:VAL:HG21 | 1:B:120:ILE:HG12 | 2 | 0.16 |
| (1,2715) | 1:B:111:VAL:HG22 | 1:B:120:ILE:HG12 | 2 | 0.16 |
| (1,2715) | 1:B:111:VAL:HG23 | 1:B:120:ILE:HG12 | 2 | 0.16 |
| (1,2715) | 1:B:111:VAL:HG11 | 1:B:120:ILE:HG12 | 2 | 0.16 |
| (1,2715) | 1:B:111:VAL:HG12 | 1:B:120:ILE:HG12 | 2 | 0.16 |
| (1,2715) | 1:B:111:VAL:HG13 | 1:B:120:ILE:HG12 | 2 | 0.16 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 4 | 0.16 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 4 | 0.16 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 4 | 0.16 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG2 | 2 | 0.16 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG3 | 2 | 0.16 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 1 | 0.16 |
| (1,2630) | 1:B:109:LEU:HA | 1:B:109:LEU:HB2 | 4 | 0.16 |
| (1,2627) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HG3 | 6 | 0.16 |
| (1,2627) | 1:B:108:GLU:HG3 | 1:B:123:LYS:HG2 | 6 | 0.16 |
| (1,258) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HA | 5 | 0.16 |
| (1,258) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HA | 5 | 0.16 |
| (1,258) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HA | 5 | 0.16 |
| (1,258) | 1:A:99:LEU:HD21 | 1:A:120:ILE:HA | 5 | 0.16 |
| (1,258) | 1:A:99:LEU:HD22 | 1:A:120:ILE:HA | 5 | 0.16 |
| (1,258) | 1:A:99:LEU:HD23 | 1:A:120:ILE:HA | 5 | 0.16 |
| (1,2577) | 1:B:105:ALA:HB1 | 1:B:107:ASP:HB2 | 2 | 0.16 |
| (1,2577) | 1:B:105:ALA:HB2 | 1:B:107:ASP:HB2 | 2 | 0.16 |
| (1,2577) | 1:B:105:ALA:HB3 | 1:B:107:ASP:HB2 | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2474) | 1:B:98:SER:HB3 | 1:B:162:THR:HA | 3 | 0.16 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD1 | 7 | 0.16 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD2 | 7 | 0.16 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD1 | 7 | 0.16 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD2 | 7 | 0.16 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD1 | 7 | 0.16 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD2 | 7 | 0.16 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG21 | 5 | 0.16 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG22 | 5 | 0.16 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG23 | 5 | 0.16 |
| (1,2383) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HB3 | 10 | 0.16 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG21 | 5 | 0.16 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG22 | 5 | 0.16 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG23 | 5 | 0.16 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD3 | 2 | 0.16 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD2 | 2 | 0.16 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 9 | 0.16 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 9 | 0.16 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 9 | 0.16 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 9 | 0.16 |
| (1,2194) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 8 | 0.16 |
| (1,2160) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB3 | 6 | 0.16 |
| (1,2160) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB3 | 9 | 0.16 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 9 | 0.16 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 9 | 0.16 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 9 | 0.16 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 9 | 0.16 |
| (1,2062) | 1:B:134:ILE:HA | 1:A:140:ARG:HD3 | 8 | 0.16 |
| (1,2028) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB3 | 6 | 0.16 |
| (1,2028) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB3 | 9 | 0.16 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 5 | 0.16 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 5 | 0.16 |
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 4 | 0.16 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 8 | 0.16 |
| (1,1964) | 1:A:166:GLU:H | 1:A:155:SER:HB2 | 6 | 0.16 |
| (1,1964) | 1:A:166:GLU:H | 1:A:155:SER:HB3 | 6 | 0.16 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 7 | 0.16 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 7 | 0.16 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 7 | 0.16 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 7 | 0.16 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 7 | 0.16 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 2 | 0.16 |
| (1,1901) | 1:A:161:GLY:H | 1:A:102:ASN:HB2 | 5 | 0.16 |
| (1,1806) | 1:A:152:GLN:HE22 | 1:A:149:ASP:HB2 | 10 | 0.16 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 3 | 0.16 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 3 | 0.16 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 3 | 0.16 |
| (1,1668) | 1:A:135:SER:H | 1:A:135:SER:HB3 | 3 | 0.16 |
| (1,1654) | 1:A:134:ILE:H | 1:A:127:ARG:HB2 | 5 | 0.16 |
| (1,1647) | 1:A:132:GLY:H | 1:A:131:HIS:HB3 | 3 | 0.16 |
| (1,1618) | 1:A:128:GLN:HE21 | 1:A:129:ASP:H | 1 | 0.16 |
| (1,1606) | 1:A:128:GLN:H | 1:A:133:TYR:HD1 | 8 | 0.16 |
| (1,1606) | 1:A:128:GLN:H | 1:A:133:TYR:HD2 | 8 | 0.16 |
| (1,1588) | 1:A:126:GLU:H | 1:A:125:GLU:HG3 | 10 | 0.16 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 2 | 0.16 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG21 | 3 | 0.16 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG22 | 3 | 0.16 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG23 | 3 | 0.16 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG11 | 3 | 0.16 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG12 | 3 | 0.16 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG13 | 3 | 0.16 |
| (1,154) | 1:A:97:VAL:HG21 | 1:A:142:TYR:HE1 | 8 | 0.16 |
| (1,154) | 1:A:97:VAL:HG21 | 1:A:142:TYR:HE2 | 8 | 0.16 |
| (1,154) | 1:A:97:VAL:HG22 | 1:A:142:TYR:HE1 | 8 | 0.16 |
| (1,154) | 1:A:97:VAL:HG22 | 1:A:142:TYR:HE2 | 8 | 0.16 |
| (1,154) | 1:A:97:VAL:HG23 | 1:A:142:TYR:HE1 | 8 | 0.16 |
| (1,154) | 1:A:97:VAL:HG23 | 1:A:142:TYR:HE2 | 8 | 0.16 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 1 | 0.16 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 1 | 0.16 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 1 | 0.16 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 1 | 0.16 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 1 | 0.16 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 1 | 0.16 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB2 | 5 | 0.16 |
| (1,15) | 1:A:93:ASP:HA | 1:A:94:ARG:HB3 | 5 | 0.16 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 9 | 0.16 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB2 | 1 | 0.16 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB3 | 1 | 0.16 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB2 | 4 | 0.16 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB3 | 4 | 0.16 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 8 | 0.16 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD21 | 8 | 0.16 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD22 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD23 | 8 | 0.16 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD21 | 8 | 0.16 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD22 | 8 | 0.16 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD23 | 8 | 0.16 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD21 | 2 | 0.16 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD22 | 2 | 0.16 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD23 | 2 | 0.16 |
| (1,1382) | 1:A:102:ASN:HD22 | 1:A:161:GLY:HA2 | 8 | 0.16 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG21 | 5 | 0.16 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG22 | 5 | 0.16 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG23 | 5 | 0.16 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 7 | 0.16 |
| (1,1277) | 1:A:168:PRO:HA | 1:A:169:MET:HG3 | 7 | 0.16 |
| (1,1258) | 1:A:166:GLU:HG2 | 1:A:167:ALA:HA | 9 | 0.16 |
| (1,1258) | 1:A:166:GLU:HG3 | 1:A:167:ALA:HA | 9 | 0.16 |
| (1,1181) | 1:A:158:SER:HA | 1:A:158:SER:HB2 | 2 | 0.16 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 2 | 0.16 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 2 | 0.16 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 2 | 0.16 |
| (1,1172) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB2 | 8 | 0.16 |
| (1,1172) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB2 | 8 | 0.16 |
| (1,1172) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB2 | 8 | 0.16 |
| (1,1149) | 1:A:157:LEU:HA | 1:A:163:LEU:HB3 | 8 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD11 | 1 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD12 | 1 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD13 | 1 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD21 | 1 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD22 | 1 | 0.16 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD23 | 1 | 0.16 |
| (1,1079) | 1:A:153:VAL:HB | 1:A:154:SER:HA | 2 | 0.16 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 2 | 0.16 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 3 | 0.16 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 4 | 0.16 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 7 | 0.16 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 8 | 0.16 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 9 | 0.16 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 10 | 0.16 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 1 | 0.16 |
| (1,101) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HA | 2 | 0.16 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG21 | 5 | 0.16 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG22 | 5 | 0.16 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG23 | 5 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 5 | 0.15 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 5 | 0.15 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 5 | 0.15 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG11 | 9 | 0.15 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG12 | 9 | 0.15 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG13 | 9 | 0.15 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG11 | 9 | 0.15 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG12 | 9 | 0.15 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG13 | 9 | 0.15 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 7 | 0.15 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 7 | 0.15 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 7 | 0.15 |
| (1,862) | 1:A:141:LYS:HG3 | 1:A:142:TYR:HB3 | 6 | 0.15 |
| (1,816) | 1:A:137:CYS:HA | 1:A:138:PHE:HD1 | 8 | 0.15 |
| (1,816) | 1:A:137:CYS:HA | 1:A:138:PHE:HD2 | 8 | 0.15 |
| (1,779) | 1:A:131:HIS:HA | 1:A:131:HIS:HE1 | 3 | 0.15 |
| (1,772) | 1:A:130:GLU:HA | 1:A:130:GLU:HG2 | 4 | 0.15 |
| (1,76) | 1:A:95:TRP:HE3 | 1:A:166:GLU:HA | 10 | 0.15 |
| (1,734) | 1:A:127:ARG:HA | 1:A:127:ARG:HB3 | 2 | 0.15 |
| (1,717) | 1:A:126:GLU:HG2 | 1:A:127:ARG:HG3 | 9 | 0.15 |
| (1,71) | 1:A:95:TRP:HB2 | 1:A:168:PRO:HB2 | 9 | 0.15 |
| (1,71) | 1:A:95:TRP:HB3 | 1:A:168:PRO:HB2 | 9 | 0.15 |
| (1,700) | 1:A:125:GLU:HA | 1:A:125:GLU:HG3 | 5 | 0.15 |
| (1,699) | 1:A:125:GLU:HA | 1:A:125:GLU:HG2 | 8 | 0.15 |
| (1,680) | 1:A:123:LYS:HA | 1:A:123:LYS:HG3 | 6 | 0.15 |
| (1,664) | 1:A:121:THR:HA | 1:A:139:THR:HA | 5 | 0.15 |
| (1,664) | 1:A:121:THR:HA | 1:A:139:THR:HA | 7 | 0.15 |
| (1,660) | 1:A:120:ILE:HD11 | 1:A:163:LEU:HD11 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD11 | 1:A:163:LEU:HD12 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD11 | 1:A:163:LEU:HD13 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD12 | 1:A:163:LEU:HD11 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD12 | 1:A:163:LEU:HD12 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD12 | 1:A:163:LEU:HD13 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD13 | 1:A:163:LEU:HD11 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD13 | 1:A:163:LEU:HD12 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD13 | 1:A:163:LEU:HD13 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD11 | 1:A:163:LEU:HD21 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD11 | 1:A:163:LEU:HD22 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD11 | 1:A:163:LEU:HD23 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD12 | 1:A:163:LEU:HD21 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD12 | 1:A:163:LEU:HD22 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD12 | 1:A:163:LEU:HD23 | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,660) | 1:A:120:ILE:HD13 | 1:A:163:LEU:HD21 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD13 | 1:A:163:LEU:HD22 | 2 | 0.15 |
| (1,660) | 1:A:120:ILE:HD13 | 1:A:163:LEU:HD23 | 2 | 0.15 |
| (1,652) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HB2 | 6 | 0.15 |
| (1,652) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HB2 | 6 | 0.15 |
| (1,652) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HB2 | 6 | 0.15 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 9 | 0.15 |
| (1,637) | 1:A:120:ILE:HB | 1:A:142:TYR:HE1 | 10 | 0.15 |
| (1,637) | 1:A:120:ILE:HB | 1:A:142:TYR:HE2 | 10 | 0.15 |
| (1,610) | 1:A:119:GLU:HA | 1:A:141:LYS:HD3 | 9 | 0.15 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 7 | 0.15 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 7 | 0.15 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 7 | 0.15 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 7 | 0.15 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 7 | 0.15 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 7 | 0.15 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD21 | 6 | 0.15 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD22 | 6 | 0.15 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD23 | 6 | 0.15 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG21 | 9 | 0.15 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG22 | 9 | 0.15 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG23 | 9 | 0.15 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 6 | 0.15 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 6 | 0.15 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 6 | 0.15 |
| (1,465) | 1:A:112:LYS:HG2 | 1:A:118:VAL:HA | 5 | 0.15 |
| (1,465) | 1:A:112:LYS:HG3 | 1:A:118:VAL:HA | 5 | 0.15 |
| (1,439) | 1:A:111:VAL:HG21 | 1:A:155:SER:HB2 | 10 | 0.15 |
| (1,439) | 1:A:111:VAL:HG22 | 1:A:155:SER:HB2 | 10 | 0.15 |
| (1,439) | 1:A:111:VAL:HG23 | 1:A:155:SER:HB2 | 10 | 0.15 |
| (1,439) | 1:A:111:VAL:HG11 | 1:A:155:SER:HB2 | 10 | 0.15 |
| (1,439) | 1:A:111:VAL:HG12 | 1:A:155:SER:HB2 | 10 | 0.15 |
| (1,439) | 1:A:111:VAL:HG13 | 1:A:155:SER:HB2 | 10 | 0.15 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 2 | 0.15 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 2 | 0.15 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 2 | 0.15 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 2 | 0.15 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 2 | 0.15 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 2 | 0.15 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 2 | 0.15 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 7 | 0.15 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 1 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD11 | 3 | 0.15 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD12 | 3 | 0.15 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD13 | 3 | 0.15 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD21 | 3 | 0.15 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD22 | 3 | 0.15 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD23 | 3 | 0.15 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG11 | 8 | 0.15 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG12 | 8 | 0.15 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG13 | 8 | 0.15 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG21 | 8 | 0.15 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG22 | 8 | 0.15 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG23 | 8 | 0.15 |
| (1,4128) | 1:B:155:SER:H | 1:B:154:SER:HB2 | 5 | 0.15 |
| (1,4115) | 1:B:154:SER:H | 1:B:155:SER:HB2 | 6 | 0.15 |
| (1,4095) | 1:B:152:GLN:HE22 | 1:B:170:PRO:HD2 | 2 | 0.15 |
| (1,4095) | 1:B:152:GLN:HE22 | 1:B:170:PRO:HD3 | 2 | 0.15 |
| (1,4077) | 1:B:152:GLN:HE21 | 1:B:149:ASP:HB2 | 6 | 0.15 |
| (1,4076) | 1:B:152:GLN:H | 1:B:170:PRO:HD2 | 2 | 0.15 |
| (1,4076) | 1:B:152:GLN:H | 1:B:170:PRO:HD3 | 2 | 0.15 |
| (1,4038) | 1:B:148:VAL:H | 1:B:170:PRO:HD2 | 6 | 0.15 |
| (1,4038) | 1:B:148:VAL:H | 1:B:170:PRO:HD3 | 6 | 0.15 |
| (1,4034) | 1:B:148:VAL:H | 1:B:149:ASP:H | 6 | 0.15 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD11 | 9 | 0.15 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD12 | 9 | 0.15 |
| (1,4007) | 1:B:144:LEU:H | 1:B:144:LEU:HD13 | 9 | 0.15 |
| (1,3955) | 1:B:137:CYS:H | 1:B:136:ARG:HB3 | 7 | 0.15 |
| (1,395) | 1:A:110:THR:HB | 1:A:112:LYS:HG2 | 2 | 0.15 |
| (1,395) | 1:A:110:THR:HB | 1:A:112:LYS:HG3 | 2 | 0.15 |
| (1,3936) | 1:B:134:ILE:H | 1:B:127:ARG:HG2 | 4 | 0.15 |
| (1,3936) | 1:B:134:ILE:H | 1:B:127:ARG:HG2 | 5 | 0.15 |
| (1,3907) | 1:B:129:ASP:H | 1:B:132:GLY:HA3 | 5 | 0.15 |
| (1,3894) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HA | 9 | 0.15 |
| (1,3889) | 1:B:128:GLN:HE22 | 1:B:128:GLN:HB2 | 3 | 0.15 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD1 | 9 | 0.15 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD2 | 9 | 0.15 |
| (1,3872) | 1:B:126:GLU:H | 1:B:135:SER:HB2 | 2 | 0.15 |
| (1,3872) | 1:B:126:GLU:H | 1:B:135:SER:HB3 | 2 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 7 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 7 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 7 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 7 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 7 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 8 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 8 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 8 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 8 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 8 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 8 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 10 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 10 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 10 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 10 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 10 | 0.15 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 10 | 0.15 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 6 | 0.15 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 6 | 0.15 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 6 | 0.15 |
| (1,383) | 1:A:109:LEU:HD21 | 1:A:122:GLY:HA3 | 10 | 0.15 |
| (1,383) | 1:A:109:LEU:HD22 | 1:A:122:GLY:HA3 | 10 | 0.15 |
| (1,383) | 1:A:109:LEU:HD23 | 1:A:122:GLY:HA3 | 10 | 0.15 |
| (1,3826) | 1:B:120:ILE:H | 1:B:140:ARG:HG3 | 8 | 0.15 |
| (1,3781) | 1:B:117:VAL:H | 1:B:115:ASP:HB2 | 6 | 0.15 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB2 | 1 | 0.15 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB3 | 1 | 0.15 |
| (1,3739) | 1:B:112:LYS:H | 1:B:112:LYS:HB3 | 2 | 0.15 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 10 | 0.15 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 10 | 0.15 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 10 | 0.15 |
| (1,3726) | 1:B:111:VAL:H | 1:B:110:THR:HB | 4 | 0.15 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 7 | 0.15 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 7 | 0.15 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 7 | 0.15 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 7 | 0.15 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 7 | 0.15 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 7 | 0.15 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 7 | 0.15 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 7 | 0.15 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 7 | 0.15 |
| (1,3672) | 1:B:105:ALA:H | 1:B:108:GLU:HB3 | 4 | 0.15 |
| (1,3664) | 1:B:102:ASN:HD22 | 1:B:161:GLY:HA3 | 6 | 0.15 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD11 | 8 | 0.15 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD12 | 8 | 0.15 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD13 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 2 | 0.15 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 2 | 0.15 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 2 | 0.15 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 2 | 0.15 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 2 | 0.15 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 2 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD21 | 4 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD22 | 4 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD23 | 4 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD21 | 6 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD22 | 6 | 0.15 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD23 | 6 | 0.15 |
| (1,3608) | 1:B:94:ARG:H | 1:B:169:MET:HG2 | 10 | 0.15 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG21 | 8 | 0.15 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG22 | 8 | 0.15 |
| (1,3600) | 1:B:94:ARG:H | 1:B:91:THR:HG23 | 8 | 0.15 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 9 | 0.15 |
| (1,3557) | 1:B:168:PRO:HA | 1:B:169:MET:HG2 | 6 | 0.15 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD2 | 5 | 0.15 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD2 | 5 | 0.15 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD3 | 5 | 0.15 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD3 | 5 | 0.15 |
| (1,3539) | 1:B:166:GLU:HG2 | 1:B:167:ALA:HA | 2 | 0.15 |
| (1,3539) | 1:B:166:GLU:HG3 | 1:B:167:ALA:HA | 2 | 0.15 |
| (1,3499) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HD21 | 7 | 0.15 |
| (1,3499) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HD22 | 7 | 0.15 |
| (1,3499) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HD23 | 7 | 0.15 |
| (1,3499) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HD11 | 7 | 0.15 |
| (1,3499) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HD12 | 7 | 0.15 |
| (1,3499) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HD13 | 7 | 0.15 |
| (1,3498) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HA | 7 | 0.15 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 6 | 0.15 |
| (1,3479) | 1:B:159:PRO:HA | 1:B:159:PRO:HB3 | 4 | 0.15 |
| (1,3453) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB2 | 5 | 0.15 |
| (1,3453) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB2 | 5 | 0.15 |
| (1,3453) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB2 | 5 | 0.15 |
| (1,3444) | 1:B:157:LEU:HG | 1:B:161:GLY:HA3 | 3 | 0.15 |
| (1,3438) | 1:B:157:LEU:HB3 | 1:B:157:LEU:HG | 9 | 0.15 |
| (1,3430) | 1:B:157:LEU:HA | 1:B:163:LEU:HB3 | 2 | 0.15 |
| (1,3430) | 1:B:157:LEU:HA | 1:B:163:LEU:HB3 | 3 | 0.15 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD21 | 3 | 0.15 |
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD22 | 3 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3421) | 1:B:156:SER:HB3 | 1:B:157:LEU:HD23 | 3 | 0.15 |
| (1,3391) | 1:B:155:SER:HA | 1:B:165:VAL:HA | 6 | 0.15 |
| (1,3366) | 1:B:153:VAL:HG11 | 1:B:155:SER:HB3 | 7 | 0.15 |
| (1,3366) | 1:B:153:VAL:HG12 | 1:B:155:SER:HB3 | 7 | 0.15 |
| (1,3366) | 1:B:153:VAL:HG13 | 1:B:155:SER:HB3 | 7 | 0.15 |
| (1,3366) | 1:B:153:VAL:HG21 | 1:B:155:SER:HB3 | 7 | 0.15 |
| (1,3366) | 1:B:153:VAL:HG22 | 1:B:155:SER:HB3 | 7 | 0.15 |
| (1,3366) | 1:B:153:VAL:HG23 | 1:B:155:SER:HB3 | 7 | 0.15 |
| (1,3358) | 1:B:153:VAL:HA | 1:B:168:PRO:HD2 | 4 | 0.15 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 5 | 0.15 |
| (1,3270) | 1:B:148:VAL:HA | 1:B:169:MET:HA | 5 | 0.15 |
| (1,3266) | 1:B:148:VAL:HA | 1:B:149:ASP:HB3 | 1 | 0.15 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 8 | 0.15 |
| (1,3143) | 1:B:141:LYS:HG3 | 1:B:142:TYR:HB3 | 9 | 0.15 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 9 | 0.15 |
| (1,3087) | 1:B:134:ILE:HG21 | 1:B:135:SER:HB3 | 8 | 0.15 |
| (1,3087) | 1:B:134:ILE:HG22 | 1:B:135:SER:HB3 | 8 | 0.15 |
| (1,3087) | 1:B:134:ILE:HG23 | 1:B:135:SER:HB3 | 8 | 0.15 |
| (1,3087) | 1:B:134:ILE:HD11 | 1:B:135:SER:HB3 | 8 | 0.15 |
| (1,3087) | 1:B:134:ILE:HD12 | 1:B:135:SER:HB3 | 8 | 0.15 |
| (1,3087) | 1:B:134:ILE:HD13 | 1:B:135:SER:HB3 | 8 | 0.15 |
| (1,3063) | 1:B:131:HIS:HB2 | 1:B:132:GLY:HA2 | 10 | 0.15 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE1 | 1 | 0.15 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE2 | 1 | 0.15 |
| (1,3018) | 1:B:127:ARG:HA | 1:B:127:ARG:HD3 | 4 | 0.15 |
| (1,3018) | 1:B:127:ARG:HA | 1:B:127:ARG:HD3 | 6 | 0.15 |
| (1,3005) | 1:B:126:GLU:HG2 | 1:B:135:SER:HB3 | 1 | 0.15 |
| (1,298) | 1:A:105:ALA:HB1 | 1:A:108:GLU:HB2 | 6 | 0.15 |
| (1,298) | 1:A:105:ALA:HB2 | 1:A:108:GLU:HB2 | 6 | 0.15 |
| (1,298) | 1:A:105:ALA:HB3 | 1:A:108:GLU:HB2 | 6 | 0.15 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 4 | 0.15 |
| (1,2945) | 1:B:121:THR:HA | 1:B:139:THR:HA | 9 | 0.15 |
| (1,2929) | 1:B:120:ILE:HG21 | 1:B:139:THR:HA | 4 | 0.15 |
| (1,2929) | 1:B:120:ILE:HG22 | 1:B:139:THR:HA | 4 | 0.15 |
| (1,2929) | 1:B:120:ILE:HG23 | 1:B:139:THR:HA | 4 | 0.15 |
| (1,2929) | 1:B:120:ILE:HG21 | 1:B:139:THR:HA | 7 | 0.15 |
| (1,2929) | 1:B:120:ILE:HG22 | 1:B:139:THR:HA | 7 | 0.15 |
| (1,2929) | 1:B:120:ILE:HG23 | 1:B:139:THR:HA | 7 | 0.15 |
| (1,2928) | 1:B:120:ILE:HG21 | 1:B:122:GLY:HA3 | 10 | 0.15 |
| (1,2928) | 1:B:120:ILE:HG22 | 1:B:122:GLY:HA3 | 10 | 0.15 |
| (1,2928) | 1:B:120:ILE:HG23 | 1:B:122:GLY:HA3 | 10 | 0.15 |
| (1,2918) | 1:B:120:ILE:HB | 1:B:142:TYR:HE1 | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2918) | 1:B:120:ILE:HB | 1:B:142:TYR:HE2 | 10 | 0.15 |
| (1,2900) | 1:B:119:GLU:HG2 | 1:B:141:LYS:HE3 | 2 | 0.15 |
| (1,2889) | 1:B:119:GLU:HA | 1:B:141:LYS:HA | 3 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 2 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 6 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 10 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 10 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 10 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 10 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 10 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 10 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 10 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 10 | 0.15 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 10 | 0.15 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG11 | 4 | 0.15 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG12 | 4 | 0.15 |
| (1,2832) | 1:B:117:VAL:HA | 1:B:148:VAL:HG13 | 4 | 0.15 |
| (1,2831) | 1:B:117:VAL:HA | 1:B:148:VAL:HB | 10 | 0.15 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG11 | 1 | 0.15 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG12 | 1 | 0.15 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG13 | 1 | 0.15 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG11 | 8 | 0.15 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG12 | 8 | 0.15 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG13 | 8 | 0.15 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG21 | 3 | 0.15 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG22 | 3 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG23 | 3 | 0.15 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG11 | 10 | 0.15 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG12 | 10 | 0.15 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG13 | 10 | 0.15 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG21 | 10 | 0.15 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG22 | 10 | 0.15 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG23 | 10 | 0.15 |
| (1,2756) | 1:B:112:LYS:HE2 | 1:B:119:GLU:HG2 | 2 | 0.15 |
| (1,2756) | 1:B:112:LYS:HE3 | 1:B:119:GLU:HG2 | 2 | 0.15 |
| (1,2752) | 1:B:112:LYS:HD2 | 1:B:114:LYS:HA | 7 | 0.15 |
| (1,2752) | 1:B:112:LYS:HD3 | 1:B:114:LYS:HA | 7 | 0.15 |
| (1,2738) | 1:B:112:LYS:HB2 | 1:B:120:ILE:HA | 7 | 0.15 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 4 | 0.15 |
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 4 | 0.15 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 4 | 0.15 |
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 4 | 0.15 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 4 | 0.15 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 4 | 0.15 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 9 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 4 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 4 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 4 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 4 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 4 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 4 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 4 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 4 | 0.15 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 4 | 0.15 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 7 | 0.15 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 4 | 0.15 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 4 | 0.15 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 4 | 0.15 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 4 | 0.15 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 4 | 0.15 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 4 | 0.15 |
| (1,2592) | 1:B:106:PRO:HA | 1:B:109:LEU:HB2 | 1 | 0.15 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 4 | 0.15 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 4 | 0.15 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 4 | 0.15 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD11 | 6 | 0.15 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD12 | 6 | 0.15 |
| (1,2570) | 1:B:105:ALA:HA | 1:B:157:LEU:HD13 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD11 | 6 | 0.15 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD12 | 6 | 0.15 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD13 | 6 | 0.15 |
| (1,2540) | 1:B:100:ASP:HA | 1:B:100:ASP:HB3 | 9 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HA | 2 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HA | 2 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HA | 2 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD21 | 1:B:120:ILE:HA | 2 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD22 | 1:B:120:ILE:HA | 2 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD23 | 1:B:120:ILE:HA | 2 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HA | 4 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HA | 4 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HA | 4 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD21 | 1:B:120:ILE:HA | 4 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD22 | 1:B:120:ILE:HA | 4 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD23 | 1:B:120:ILE:HA | 4 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HA | 5 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HA | 5 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HA | 5 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD21 | 1:B:120:ILE:HA | 5 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD22 | 1:B:120:ILE:HA | 5 | 0.15 |
| (1,2539) | 1:B:99:LEU:HD23 | 1:B:120:ILE:HA | 5 | 0.15 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG3 | 9 | 0.15 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG2 | 9 | 0.15 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD3 | 5 | 0.15 |
| (1,2374) | 1:B:96:ARG:HB2 | 1:B:96:ARG:HD2 | 5 | 0.15 |
| (1,2342) | 1:B:95:TRP:HB2 | 1:B:96:ARG:HA | 8 | 0.15 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD3 | 6 | 0.15 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD2 | 6 | 0.15 |
| (1,2318) | 1:B:94:ARG:HB2 | 1:B:96:ARG:HA | 6 | 0.15 |
| (1,2304) | 1:B:94:ARG:HA | 1:B:94:ARG:HB3 | 10 | 0.15 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 3 | 0.15 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 3 | 0.15 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 3 | 0.15 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 3 | 0.15 |
| (1,2225) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 2 | 0.15 |
| (1,2225) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 2 | 0.15 |
| (1,2225) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 2 | 0.15 |
| (1,2225) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 8 | 0.15 |
| (1,2225) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 8 | 0.15 |
| (1,2225) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 8 | 0.15 |
| (1,2160) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB3 | 1 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2152) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2152) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2152) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2152) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2152) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2152) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 3 | 0.15 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 3 | 0.15 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 3 | 0.15 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 3 | 0.15 |
| (1,2093) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 2 | 0.15 |
| (1,2093) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 2 | 0.15 |
| (1,2093) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 2 | 0.15 |
| (1,2093) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 8 | 0.15 |
| (1,2093) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 8 | 0.15 |
| (1,2093) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 8 | 0.15 |
| (1,206) | 1:A:99:LEU:HA | 1:A:120:ILE:HD11 | 2 | 0.15 |
| (1,206) | 1:A:99:LEU:HA | 1:A:120:ILE:HD12 | 2 | 0.15 |
| (1,206) | 1:A:99:LEU:HA | 1:A:120:ILE:HD13 | 2 | 0.15 |
| (1,2028) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB3 | 1 | 0.15 |
| (1,2020) | 1:A:97:VAL:HG11 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2020) | 1:A:97:VAL:HG12 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2020) | 1:A:97:VAL:HG13 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2020) | 1:A:97:VAL:HG21 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2020) | 1:A:97:VAL:HG22 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,2020) | 1:A:97:VAL:HG23 | 1:B:131:HIS:HB3 | 3 | 0.15 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG2 | 3 | 0.15 |
| (1,1983) | 1:A:167:ALA:H | 1:A:166:GLU:HG3 | 3 | 0.15 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 10 | 0.15 |
| (1,1964) | 1:A:166:GLU:H | 1:A:155:SER:HB2 | 8 | 0.15 |
| (1,1964) | 1:A:166:GLU:H | 1:A:155:SER:HB3 | 8 | 0.15 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 3 | 0.15 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 3 | 0.15 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 3 | 0.15 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 3 | 0.15 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 3 | 0.15 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 3 | 0.15 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG21 | 6 | 0.15 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG22 | 6 | 0.15 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG23 | 6 | 0.15 |
| (1,1901) | 1:A:161:GLY:H | 1:A:102:ASN:HB2 | 4 | 0.15 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG21 | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG22 | 10 | 0.15 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG23 | 10 | 0.15 |
| (1,1816) | 1:A:153:VAL:H | 1:A:149:ASP:HB2 | 4 | 0.15 |
| (1,1766) | 1:A:149:ASP:H | 1:A:169:MET:HG3 | 4 | 0.15 |
| (1,1743) | 1:A:148:VAL:H | 1:A:146:PRO:HB3 | 5 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 5 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 5 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 5 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 10 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 10 | 0.15 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 10 | 0.15 |
| (1,1667) | 1:A:135:SER:H | 1:A:135:SER:HB2 | 9 | 0.15 |
| (1,1647) | 1:A:132:GLY:H | 1:A:131:HIS:HB3 | 7 | 0.15 |
| (1,1642) | 1:A:132:GLY:H | 1:A:129:ASP:HB2 | 4 | 0.15 |
| (1,1626) | 1:A:129:ASP:H | 1:A:132:GLY:HA3 | 3 | 0.15 |
| (1,1622) | 1:A:129:ASP:H | 1:A:129:ASP:HB3 | 9 | 0.15 |
| (1,1611) | 1:A:128:GLN:HE22 | 1:A:128:GLN:H | 2 | 0.15 |
| (1,1600) | 1:A:128:GLN:H | 1:A:127:ARG:HD2 | 1 | 0.15 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB1 | 7 | 0.15 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB2 | 7 | 0.15 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB3 | 7 | 0.15 |
| (1,1546) | 1:A:120:ILE:H | 1:A:142:TYR:H | 4 | 0.15 |
| (1,1517) | 1:A:118:VAL:H | 1:A:142:TYR:HB2 | 5 | 0.15 |
| (1,1509) | 1:A:117:VAL:H | 1:A:144:LEU:H | 5 | 0.15 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 6 | 0.15 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 6 | 0.15 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 6 | 0.15 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 6 | 0.15 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 6 | 0.15 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 6 | 0.15 |
| (1,1489) | 1:A:114:LYS:H | 1:A:119:GLU:H | 2 | 0.15 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG21 | 2 | 0.15 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG22 | 2 | 0.15 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG23 | 2 | 0.15 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG11 | 2 | 0.15 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG12 | 2 | 0.15 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG13 | 2 | 0.15 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD11 | 3 | 0.15 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD12 | 3 | 0.15 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD13 | 3 | 0.15 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD11 | 5 | 0.15 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD12 | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD13 | 5 | 0.15 |
| (1,1418) | 1:A:108:GLU:H | 1:A:108:GLU:HG2 | 3 | 0.15 |
| (1,1418) | 1:A:108:GLU:H | 1:A:108:GLU:HG3 | 3 | 0.15 |
| (1,1389) | 1:A:105:ALA:H | 1:A:106:PRO:HD3 | 10 | 0.15 |
| (1,1373) | 1:A:102:ASN:HD21 | 1:A:161:GLY:HA2 | 2 | 0.15 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB2 | 1 | 0.15 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB3 | 1 | 0.15 |
| (1,1345) | 1:A:97:VAL:H | 1:A:165:VAL:H | 7 | 0.15 |
| (1,1333) | 1:A:95:TRP:H | 1:A:166:GLU:HG2 | 5 | 0.15 |
| (1,1333) | 1:A:95:TRP:H | 1:A:166:GLU:HG3 | 5 | 0.15 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG21 | 2 | 0.15 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG22 | 2 | 0.15 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG23 | 2 | 0.15 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 6 | 0.15 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG2 | 2 | 0.15 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG3 | 2 | 0.15 |
| (1,1218) | 1:A:161:GLY:HA3 | 1:A:163:LEU:HD21 | 5 | 0.15 |
| (1,1218) | 1:A:161:GLY:HA3 | 1:A:163:LEU:HD22 | 5 | 0.15 |
| (1,1218) | 1:A:161:GLY:HA3 | 1:A:163:LEU:HD23 | 5 | 0.15 |
| (1,1218) | 1:A:161:GLY:HA3 | 1:A:163:LEU:HD11 | 5 | 0.15 |
| (1,1218) | 1:A:161:GLY:HA3 | 1:A:163:LEU:HD12 | 5 | 0.15 |
| (1,1218) | 1:A:161:GLY:HA3 | 1:A:163:LEU:HD13 | 5 | 0.15 |
| (1,1210) | 1:A:160:GLU:HB2 | 1:A:162:THR:HB | 6 | 0.15 |
| (1,1189) | 1:A:158:SER:HA | 1:A:160:GLU:HB3 | 5 | 0.15 |
| (1,1177) | 1:A:157:LEU:HD21 | 1:A:161:GLY:HA3 | 4 | 0.15 |
| (1,1177) | 1:A:157:LEU:HD22 | 1:A:161:GLY:HA3 | 4 | 0.15 |
| (1,1177) | 1:A:157:LEU:HD23 | 1:A:161:GLY:HA3 | 4 | 0.15 |
| (1,1157) | 1:A:157:LEU:HB3 | 1:A:157:LEU:HG | 3 | 0.15 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 8 | 0.15 |
| (1,1149) | 1:A:157:LEU:HA | 1:A:163:LEU:HB3 | 4 | 0.15 |
| (1,1148) | 1:A:157:LEU:HA | 1:A:162:THR:HB | 2 | 0.15 |
| (1,1119) | 1:A:155:SER:HB2 | 1:A:165:VAL:HA | 6 | 0.15 |
| (1,1110) | 1:A:155:SER:HA | 1:A:165:VAL:HA | 10 | 0.15 |
| (1,1035) | 1:A:150:PRO:HA | 1:A:150:PRO:HB3 | 6 | 0.15 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 5 | 0.15 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 10 | 0.15 |
| (1,992) | 1:A:148:VAL:HA | 1:A:170:PRO:HB3 | 1 | 0.14 |
| (1,977) | 1:A:147:GLY:HA3 | 1:A:148:VAL:HB | 5 | 0.14 |
| (1,917) | 1:A:144:LEU:HB3 | 1:A:147:GLY:HA2 | 9 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 1 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 1 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 2 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 2 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 2 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 3 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 3 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 3 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 10 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 10 | 0.14 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 10 | 0.14 |
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG21 | 9 | 0.14 |
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG22 | 9 | 0.14 |
| (1,883) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG23 | 9 | 0.14 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG21 | 9 | 0.14 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG22 | 9 | 0.14 |
| (1,883) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG23 | 9 | 0.14 |
| (1,857) | 1:A:141:LYS:HG2 | 1:A:143:THR:HA | 4 | 0.14 |
| (1,857) | 1:A:141:LYS:HG2 | 1:A:143:THR:HA | 6 | 0.14 |
| (1,853) | 1:A:141:LYS:HG2 | 1:A:141:LYS:HE3 | 5 | 0.14 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 10 | 0.14 |
| (1,831) | 1:A:139:THR:HB | 1:A:141:LYS:HE2 | 7 | 0.14 |
| (1,759) | 1:A:128:GLN:HG2 | 1:A:133:TYR:HA | 5 | 0.14 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD11 | 4 | 0.14 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD12 | 4 | 0.14 |
| (1,751) | 1:A:128:GLN:HA | 1:A:134:ILE:HD13 | 4 | 0.14 |
| (1,690) | 1:A:123:LYS:HB3 | 1:A:137:CYS:HB2 | 1 | 0.14 |
| (1,684) | 1:A:123:LYS:HA | 1:A:135:SER:HB3 | 1 | 0.14 |
| (1,652) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HB2 | 8 | 0.14 |
| (1,652) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HB2 | 8 | 0.14 |
| (1,652) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HB2 | 8 | 0.14 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD1 | 1 | 0.14 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD2 | 1 | 0.14 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD1 | 1 | 0.14 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD2 | 1 | 0.14 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD1 | 1 | 0.14 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD2 | 1 | 0.14 |
| (1,605) | 1:A:119:GLU:HA | 1:A:120:ILE:HG13 | 3 | 0.14 |
| (1,604) | 1:A:119:GLU:HA | 1:A:120:ILE:HG12 | 6 | 0.14 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG11 | 2 | 0.14 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG12 | 2 | 0.14 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG13 | 2 | 0.14 |
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG11 | 2 | 0.14 |
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG12 | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG13 | 2 | 0.14 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG11 | 2 | 0.14 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG12 | 2 | 0.14 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG13 | 2 | 0.14 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD1 | 3 | 0.14 |
| (1,585) | 1:A:118:VAL:HG11 | 1:A:142:TYR:HD2 | 3 | 0.14 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD1 | 3 | 0.14 |
| (1,585) | 1:A:118:VAL:HG12 | 1:A:142:TYR:HD2 | 3 | 0.14 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD1 | 3 | 0.14 |
| (1,585) | 1:A:118:VAL:HG13 | 1:A:142:TYR:HD2 | 3 | 0.14 |
| (1,571) | 1:A:118:VAL:HB | 1:A:142:TYR:HD1 | 10 | 0.14 |
| (1,571) | 1:A:118:VAL:HB | 1:A:142:TYR:HD2 | 10 | 0.14 |
| (1,558) | 1:A:117:VAL:HG11 | 1:A:141:LYS:HE2 | 6 | 0.14 |
| (1,558) | 1:A:117:VAL:HG12 | 1:A:141:LYS:HE2 | 6 | 0.14 |
| (1,558) | 1:A:117:VAL:HG13 | 1:A:141:LYS:HE2 | 6 | 0.14 |
| (1,558) | 1:A:117:VAL:HG21 | 1:A:141:LYS:HE2 | 6 | 0.14 |
| (1,558) | 1:A:117:VAL:HG22 | 1:A:141:LYS:HE2 | 6 | 0.14 |
| (1,558) | 1:A:117:VAL:HG23 | 1:A:141:LYS:HE2 | 6 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 5 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 5 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 5 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 8 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 8 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 8 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 10 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 10 | 0.14 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 10 | 0.14 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG11 | 10 | 0.14 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG12 | 10 | 0.14 |
| (1,529) | 1:A:116:GLY:HA2 | 1:A:148:VAL:HG13 | 10 | 0.14 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 7 | 0.14 |
| (1,453) | 1:A:112:LYS:HA | 1:A:114:LYS:HB3 | 10 | 0.14 |
| (1,4280) | 1:B:169:MET:H | 1:B:169:MET:HB3 | 6 | 0.14 |
| (1,4278) | 1:B:169:MET:H | 1:B:169:MET:HA | 4 | 0.14 |
| (1,4262) | 1:B:167:ALA:H | 1:B:166:GLU:HB2 | 1 | 0.14 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD11 | 10 | 0.14 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD12 | 10 | 0.14 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD13 | 10 | 0.14 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD21 | 10 | 0.14 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD22 | 10 | 0.14 |
| (1,425) | 1:A:111:VAL:HB | 1:A:163:LEU:HD23 | 10 | 0.14 |
| (1,4239) | 1:B:165:VAL:H | 1:B:166:GLU:HB3 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD11 | 9 | 0.14 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD12 | 9 | 0.14 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD13 | 9 | 0.14 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 6 | 0.14 |
| (1,4183) | 1:B:161:GLY:H | 1:B:102:ASN:HB3 | 9 | 0.14 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 5 | 0.14 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD11 | 10 | 0.14 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD12 | 10 | 0.14 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD13 | 10 | 0.14 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD21 | 10 | 0.14 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD22 | 10 | 0.14 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD23 | 10 | 0.14 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG21 | 3 | 0.14 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG22 | 3 | 0.14 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG23 | 3 | 0.14 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG21 | 5 | 0.14 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG22 | 5 | 0.14 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG23 | 5 | 0.14 |
| (1,4089) | 1:B:152:GLN:HE22 | 1:B:152:GLN:HB2 | 4 | 0.14 |
| (1,4085) | 1:B:152:GLN:HE21 | 1:B:169:MET:HA | 10 | 0.14 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 5 | 0.14 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 5 | 0.14 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 5 | 0.14 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 6 | 0.14 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 6 | 0.14 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 6 | 0.14 |
| (1,4075) | 1:B:152:GLN:H | 1:B:168:PRO:HD3 | 5 | 0.14 |
| (1,4033) | 1:B:148:VAL:H | 1:B:149:ASP:HB2 | 1 | 0.14 |
| (1,3936) | 1:B:134:ILE:H | 1:B:127:ARG:HG2 | 1 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG21 | 8 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG22 | 8 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG23 | 8 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG11 | 8 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG12 | 8 | 0.14 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG13 | 8 | 0.14 |
| (1,3915) | 1:B:131:HIS:H | 1:B:129:ASP:HB3 | 3 | 0.14 |
| (1,3910) | 1:B:129:ASP:H | 1:B:133:TYR:HB2 | 2 | 0.14 |
| (1,3894) | 1:B:128:GLN:HE21 | 1:B:128:GLN:HA | 3 | 0.14 |
| (1,3879) | 1:B:128:GLN:H | 1:B:127:ARG:HG2 | 3 | 0.14 |
| (1,3869) | 1:B:126:GLU:H | 1:B:125:GLU:HG3 | 8 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG21 | 2 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG22 | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG23 | 2 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG11 | 2 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG12 | 2 | 0.14 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG13 | 2 | 0.14 |
| (1,3733) | 1:B:112:LYS:H | 1:B:99:LEU:HD21 | 2 | 0.14 |
| (1,3733) | 1:B:112:LYS:H | 1:B:99:LEU:HD22 | 2 | 0.14 |
| (1,3733) | 1:B:112:LYS:H | 1:B:99:LEU:HD23 | 2 | 0.14 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD11 | 9 | 0.14 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD12 | 9 | 0.14 |
| (1,3730) | 1:B:111:VAL:H | 1:B:120:ILE:HD13 | 9 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 1 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 4 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 5 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 5 | 0.14 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 5 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 5 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 5 | 0.14 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 5 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 5 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 5 | 0.14 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 5 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 8 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 8 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 8 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 8 | 0.14 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 8 | 0.14 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD11 | 2 | 0.14 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD12 | 2 | 0.14 |
| (1,3666) | 1:B:103:HIS:H | 1:B:157:LEU:HD13 | 2 | 0.14 |
| (1,3654) | 1:B:102:ASN:HD21 | 1:B:161:GLY:HA2 | 8 | 0.14 |
| (1,3614) | 1:B:95:TRP:H | 1:B:166:GLU:HG2 | 3 | 0.14 |
| (1,3614) | 1:B:95:TRP:H | 1:B:166:GLU:HG3 | 3 | 0.14 |
| (1,3614) | 1:B:95:TRP:H | 1:B:166:GLU:HG2 | 5 | 0.14 |
| (1,3614) | 1:B:95:TRP:H | 1:B:166:GLU:HG3 | 5 | 0.14 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 5 | 0.14 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 8 | 0.14 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 2 | 0.14 |
| (1,3453) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB2 | 8 | 0.14 |
| (1,3453) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB2 | 8 | 0.14 |
| (1,3453) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB2 | 8 | 0.14 |
| (1,3449) | 1:B:157:LEU:HD11 | 1:B:161:GLY:HA3 | 9 | 0.14 |
| (1,3449) | 1:B:157:LEU:HD12 | 1:B:161:GLY:HA3 | 9 | 0.14 |
| (1,3449) | 1:B:157:LEU:HD13 | 1:B:161:GLY:HA3 | 9 | 0.14 |
| (1,344) | 1:A:108:GLU:HG2 | 1:A:123:LYS:HD3 | 8 | 0.14 |
| (1,344) | 1:A:108:GLU:HG2 | 1:A:123:LYS:HD2 | 8 | 0.14 |
| (1,3438) | 1:B:157:LEU:HB3 | 1:B:157:LEU:HG | 6 | 0.14 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD11 | 7 | 0.14 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD12 | 7 | 0.14 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD13 | 7 | 0.14 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD21 | 7 | 0.14 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD22 | 7 | 0.14 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD23 | 7 | 0.14 |
| (1,3360) | 1:B:153:VAL:HB | 1:B:154:SER:HA | 10 | 0.14 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD21 | 9 | 0.14 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD22 | 9 | 0.14 |
| (1,335) | 1:A:107:ASP:HA | 1:A:157:LEU:HD23 | 9 | 0.14 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG21 | 2 | 0.14 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG22 | 2 | 0.14 |
| (1,3317) | 1:B:150:PRO:HA | 1:B:151:THR:HG23 | 2 | 0.14 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 1 | 0.14 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 3 | 0.14 |
| (1,3316) | 1:B:150:PRO:HA | 1:B:150:PRO:HB3 | 7 | 0.14 |
| (1,3301) | 1:B:148:VAL:HG21 | 1:B:169:MET:HB2 | 2 | 0.14 |
| (1,3301) | 1:B:148:VAL:HG22 | 1:B:169:MET:HB2 | 2 | 0.14 |
| (1,3301) | 1:B:148:VAL:HG23 | 1:B:169:MET:HB2 | 2 | 0.14 |
| (1,3278) | 1:B:148:VAL:HB | 1:B:150:PRO:HA | 4 | 0.14 |
| (1,3274) | 1:B:148:VAL:HA | 1:B:170:PRO:HG2 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 7 | 0.14 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 7 | 0.14 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 7 | 0.14 |
| (1,3123) | 1:B:141:LYS:HA | 1:B:141:LYS:HB2 | 10 | 0.14 |
| (1,3024) | 1:B:127:ARG:HB3 | 1:B:127:ARG:HD2 | 9 | 0.14 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD11 | 3 | 0.14 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD12 | 3 | 0.14 |
| (1,3022) | 1:B:127:ARG:HA | 1:B:134:ILE:HD13 | 3 | 0.14 |
| (1,3) | 1:A:89:ARG:HB2 | 1:A:90:HIS:HB2 | 9 | 0.14 |
| (1,3) | 1:A:89:ARG:HB3 | 1:A:90:HIS:HB2 | 9 | 0.14 |
| (1,2989) | 1:B:126:GLU:HA | 1:B:134:ILE:HG21 | 7 | 0.14 |
| (1,2989) | 1:B:126:GLU:HA | 1:B:134:ILE:HG22 | 7 | 0.14 |
| (1,2989) | 1:B:126:GLU:HA | 1:B:134:ILE:HG23 | 7 | 0.14 |
| (1,2918) | 1:B:120:ILE:HB | 1:B:142:TYR:HE1 | 1 | 0.14 |
| (1,2918) | 1:B:120:ILE:HB | 1:B:142:TYR:HE2 | 1 | 0.14 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 9 | 0.14 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 9 | 0.14 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 9 | 0.14 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 10 | 0.14 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 10 | 0.14 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 10 | 0.14 |
| (1,2883) | 1:B:119:GLU:HA | 1:B:119:GLU:HG3 | 8 | 0.14 |
| (1,2883) | 1:B:119:GLU:HA | 1:B:119:GLU:HG3 | 10 | 0.14 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG21 | 2 | 0.14 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG22 | 2 | 0.14 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG23 | 2 | 0.14 |
| (1,2799) | 1:B:115:ASP:HB3 | 1:B:150:PRO:HG3 | 2 | 0.14 |
| (1,2791) | 1:B:114:LYS:HB2 | 1:B:118:VAL:HA | 7 | 0.14 |
| (1,2791) | 1:B:114:LYS:HB3 | 1:B:118:VAL:HA | 7 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG11 | 5 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG12 | 5 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG13 | 5 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG21 | 5 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG22 | 5 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG23 | 5 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG11 | 6 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG12 | 6 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG13 | 6 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG21 | 6 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG22 | 6 | 0.14 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG23 | 6 | 0.14 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 7 | 0.14 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 7 | 0.14 |
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 7 | 0.14 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 7 | 0.14 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 7 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD11 | 2 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD12 | 2 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD13 | 2 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD21 | 2 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD22 | 2 | 0.14 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD23 | 2 | 0.14 |
| (1,2704) | 1:B:111:VAL:HB | 1:B:112:LYS:HA | 5 | 0.14 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 8 | 0.14 |
| (1,2685) | 1:B:110:THR:HG21 | 1:B:112:LYS:HB2 | 1 | 0.14 |
| (1,2685) | 1:B:110:THR:HG22 | 1:B:112:LYS:HB2 | 1 | 0.14 |
| (1,2685) | 1:B:110:THR:HG23 | 1:B:112:LYS:HB2 | 1 | 0.14 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG2 | 3 | 0.14 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG3 | 3 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 2 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 2 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 2 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 2 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 2 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 2 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 3 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 3 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 3 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 3 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 3 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 3 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 4 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 4 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 4 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 4 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 4 | 0.14 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 4 | 0.14 |
| (1,2654) | 1:B:109:LEU:HD11 | 1:B:161:GLY:HA3 | 4 | 0.14 |
| (1,2654) | 1:B:109:LEU:HD12 | 1:B:161:GLY:HA3 | 4 | 0.14 |
| (1,2654) | 1:B:109:LEU:HD13 | 1:B:161:GLY:HA3 | 4 | 0.14 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 3 | 0.14 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 3 | 0.14 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 3 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 3 | 0.14 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 3 | 0.14 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 3 | 0.14 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 3 | 0.14 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 3 | 0.14 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 3 | 0.14 |
| (1,265) | 1:A:100:ASP:HB3 | 1:A:162:THR:HA | 9 | 0.14 |
| (1,264) | 1:A:100:ASP:HB2 | 1:A:162:THR:HB | 4 | 0.14 |
| (1,258) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HA | 7 | 0.14 |
| (1,258) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HA | 7 | 0.14 |
| (1,258) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HA | 7 | 0.14 |
| (1,258) | 1:A:99:LEU:HD21 | 1:A:120:ILE:HA | 7 | 0.14 |
| (1,258) | 1:A:99:LEU:HD22 | 1:A:120:ILE:HA | 7 | 0.14 |
| (1,258) | 1:A:99:LEU:HD23 | 1:A:120:ILE:HA | 7 | 0.14 |
| (1,2561) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA3 | 8 | 0.14 |
| (1,2561) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA3 | 10 | 0.14 |
| (1,2560) | 1:B:102:ASN:HB3 | 1:B:161:GLY:HA2 | 2 | 0.14 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD11 | 4 | 0.14 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD12 | 4 | 0.14 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD13 | 4 | 0.14 |
| (1,2432) | 1:B:97:VAL:HG21 | 1:B:142:TYR:HB2 | 5 | 0.14 |
| (1,2432) | 1:B:97:VAL:HG22 | 1:B:142:TYR:HB2 | 5 | 0.14 |
| (1,2432) | 1:B:97:VAL:HG23 | 1:B:142:TYR:HB2 | 5 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD1 | 9 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD2 | 9 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD1 | 9 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD2 | 9 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD1 | 9 | 0.14 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD2 | 9 | 0.14 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 4 | 0.14 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 4 | 0.14 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 4 | 0.14 |
| (1,2380) | 1:B:96:ARG:HB3 | 1:B:164:THR:HB | 1 | 0.14 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG3 | 4 | 0.14 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG2 | 4 | 0.14 |
| (1,236) | 1:A:99:LEU:HD11 | 1:A:164:THR:HA | 8 | 0.14 |
| (1,236) | 1:A:99:LEU:HD12 | 1:A:164:THR:HA | 8 | 0.14 |
| (1,236) | 1:A:99:LEU:HD13 | 1:A:164:THR:HA | 8 | 0.14 |
| (1,2357) | 1:B:95:TRP:HE3 | 1:B:166:GLU:HA | 7 | 0.14 |
| (1,2325) | 1:B:94:ARG:HG2 | 1:B:166:GLU:HB2 | 6 | 0.14 |
| (1,2325) | 1:B:94:ARG:HG3 | 1:B:166:GLU:HB2 | 6 | 0.14 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD3 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD2 | 5 | 0.14 |
| (1,2310) | 1:B:94:ARG:HA | 1:B:168:PRO:HA | 1 | 0.14 |
| (1,23) | 1:A:94:ARG:HA | 1:A:94:ARG:HB3 | 7 | 0.14 |
| (1,226) | 1:A:99:LEU:HD11 | 1:A:101:VAL:HG21 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD11 | 1:A:101:VAL:HG22 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD11 | 1:A:101:VAL:HG23 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD12 | 1:A:101:VAL:HG21 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD12 | 1:A:101:VAL:HG22 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD12 | 1:A:101:VAL:HG23 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD13 | 1:A:101:VAL:HG21 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD13 | 1:A:101:VAL:HG22 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD13 | 1:A:101:VAL:HG23 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD11 | 1:A:101:VAL:HG11 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD11 | 1:A:101:VAL:HG12 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD11 | 1:A:101:VAL:HG13 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD12 | 1:A:101:VAL:HG11 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD12 | 1:A:101:VAL:HG12 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD12 | 1:A:101:VAL:HG13 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD13 | 1:A:101:VAL:HG11 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD13 | 1:A:101:VAL:HG12 | 2 | 0.14 |
| (1,226) | 1:A:99:LEU:HD13 | 1:A:101:VAL:HG13 | 2 | 0.14 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 10 | 0.14 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 10 | 0.14 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 10 | 0.14 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 10 | 0.14 |
| (1,2170) | 1:A:132:GLY:HA3 | 1:B:142:TYR:HA | 5 | 0.14 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 10 | 0.14 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 10 | 0.14 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 10 | 0.14 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 10 | 0.14 |
| (1,2038) | 1:A:132:GLY:HA3 | 1:B:142:TYR:HA | 5 | 0.14 |
| (1,203) | 1:A:99:LEU:HA | 1:A:100:ASP:HB3 | 7 | 0.14 |
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD21 | 9 | 0.14 |
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD22 | 9 | 0.14 |
| (1,201) | 1:A:99:LEU:HA | 1:A:99:LEU:HD23 | 9 | 0.14 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB2 | 6 | 0.14 |
| (1,2009) | 1:A:171:LYS:H | 1:A:171:LYS:HB3 | 6 | 0.14 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB2 | 9 | 0.14 |
| (1,2005) | 1:A:171:LYS:H | 1:A:170:PRO:HB3 | 9 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 1 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 1 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 1 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 1 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 1 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD11 | 4 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD12 | 4 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD13 | 4 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD21 | 4 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD22 | 4 | 0.14 |
| (1,1944) | 1:A:164:THR:H | 1:A:163:LEU:HD23 | 4 | 0.14 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 7 | 0.14 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 10 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD11 | 5 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD12 | 5 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD13 | 5 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD21 | 5 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD22 | 5 | 0.14 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD23 | 5 | 0.14 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG21 | 4 | 0.14 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG22 | 4 | 0.14 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG23 | 4 | 0.14 |
| (1,1877) | 1:A:158:SER:H | 1:A:109:LEU:HD11 | 2 | 0.14 |
| (1,1877) | 1:A:158:SER:H | 1:A:109:LEU:HD12 | 2 | 0.14 |
| (1,1877) | 1:A:158:SER:H | 1:A:109:LEU:HD13 | 2 | 0.14 |
| (1,1870) | 1:A:157:LEU:H | 1:A:157:LEU:HB3 | 5 | 0.14 |
| (1,1847) | 1:A:155:SER:H | 1:A:154:SER:HB2 | 3 | 0.14 |
| (1,1834) | 1:A:154:SER:H | 1:A:155:SER:HB2 | 6 | 0.14 |
| (1,1771) | 1:A:151:THR:H | 1:A:149:ASP:HB3 | 6 | 0.14 |
| (1,1762) | 1:A:149:ASP:H | 1:A:152:GLN:HB2 | 6 | 0.14 |
| (1,1743) | 1:A:148:VAL:H | 1:A:146:PRO:HB3 | 9 | 0.14 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 9 | 0.14 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 9 | 0.14 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 9 | 0.14 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 8 | 0.14 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 8 | 0.14 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 8 | 0.14 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 8 | 0.14 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 8 | 0.14 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 8 | 0.14 |
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG21 | 1 | 0.14 |
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG22 | 1 | 0.14 |
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG23 | 1 | 0.14 |
| (1,1651) | 1:A:132:GLY:H | 1:A:133:TYR:HE1 | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1651) | 1:A:132:GLY:H | 1:A:133:TYR:HE2 | 9 | 0.14 |
| (1,161) | 1:A:97:VAL:HG21 | 1:A:166:GLU:HA | 5 | 0.14 |
| (1,161) | 1:A:97:VAL:HG22 | 1:A:166:GLU:HA | 5 | 0.14 |
| (1,161) | 1:A:97:VAL:HG23 | 1:A:166:GLU:HA | 5 | 0.14 |
| (1,1606) | 1:A:128:GLN:H | 1:A:133:TYR:HD1 | 3 | 0.14 |
| (1,1606) | 1:A:128:GLN:H | 1:A:133:TYR:HD2 | 3 | 0.14 |
| (1,1581) | 1:A:125:GLU:H | 1:A:108:GLU:HG3 | 2 | 0.14 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD11 | 3 | 0.14 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD12 | 3 | 0.14 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD13 | 3 | 0.14 |
| (1,1566) | 1:A:123:LYS:H | 1:A:109:LEU:HB2 | 1 | 0.14 |
| (1,1543) | 1:A:120:ILE:H | 1:A:140:ARG:HB2 | 6 | 0.14 |
| (1,1543) | 1:A:120:ILE:H | 1:A:140:ARG:HB3 | 6 | 0.14 |
| (1,1525) | 1:A:119:GLU:H | 1:A:114:LYS:HB3 | 1 | 0.14 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG11 | 9 | 0.14 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG12 | 9 | 0.14 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG13 | 9 | 0.14 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG21 | 9 | 0.14 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG22 | 9 | 0.14 |
| (1,1506) | 1:A:117:VAL:H | 1:A:118:VAL:HG23 | 9 | 0.14 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB2 | 10 | 0.14 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB3 | 10 | 0.14 |
| (1,143) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HE1 | 7 | 0.14 |
| (1,143) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HE2 | 7 | 0.14 |
| (1,143) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HE1 | 7 | 0.14 |
| (1,143) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HE2 | 7 | 0.14 |
| (1,143) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HE1 | 7 | 0.14 |
| (1,143) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HE2 | 7 | 0.14 |
| (1,1428) | 1:A:109:LEU:H | 1:A:109:LEU:HB3 | 7 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD21 | 2 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD22 | 2 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD23 | 2 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD21 | 2 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD22 | 2 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD23 | 2 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD21 | 7 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD22 | 7 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD23 | 7 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD21 | 7 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD22 | 7 | 0.14 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD23 | 7 | 0.14 |
| (1,1400) | 1:A:107:ASP:H | 1:A:106:PRO:HB3 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1391) | 1:A:105:ALA:H | 1:A:108:GLU:HB3 | 3 | 0.14 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD11 | 6 | 0.14 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD12 | 6 | 0.14 |
| (1,1385) | 1:A:103:HIS:H | 1:A:157:LEU:HD13 | 6 | 0.14 |
| (1,1383) | 1:A:102:ASN:HD22 | 1:A:161:GLY:HA3 | 7 | 0.14 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD11 | 2 | 0.14 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD12 | 2 | 0.14 |
| (1,1371) | 1:A:102:ASN:HD21 | 1:A:157:LEU:HD13 | 2 | 0.14 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB2 | 3 | 0.14 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB3 | 3 | 0.14 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 10 | 0.14 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 10 | 0.14 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 10 | 0.14 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 10 | 0.14 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 10 | 0.14 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 10 | 0.14 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG21 | 6 | 0.14 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG22 | 6 | 0.14 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG23 | 6 | 0.14 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 8 | 0.14 |
| (1,1282) | 1:A:168:PRO:HB3 | 1:A:169:MET:HA | 3 | 0.14 |
| (1,1174) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HG | 10 | 0.14 |
| (1,1174) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HG | 10 | 0.14 |
| (1,1174) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HG | 10 | 0.14 |
| (1,117) | 1:A:96:ARG:HD2 | 1:A:166:GLU:HG2 | 7 | 0.14 |
| (1,117) | 1:A:96:ARG:HD3 | 1:A:166:GLU:HG3 | 7 | 0.14 |
| (1,117) | 1:A:96:ARG:HD3 | 1:A:166:GLU:HG2 | 7 | 0.14 |
| (1,117) | 1:A:96:ARG:HD2 | 1:A:166:GLU:HG3 | 7 | 0.14 |
| (1,1157) | 1:A:157:LEU:HB3 | 1:A:157:LEU:HG | 1 | 0.14 |
| (1,1157) | 1:A:157:LEU:HB3 | 1:A:157:LEU:HG | 2 | 0.14 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD11 | 10 | 0.14 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD12 | 10 | 0.14 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD13 | 10 | 0.14 |
| (1,1110) | 1:A:155:SER:HA | 1:A:165:VAL:HA | 7 | 0.14 |
| (1,1110) | 1:A:155:SER:HA | 1:A:165:VAL:HA | 9 | 0.14 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD11 | 2 | 0.14 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD12 | 2 | 0.14 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD13 | 2 | 0.14 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD21 | 2 | 0.14 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD22 | 2 | 0.14 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD23 | 2 | 0.14 |
| (1,1096) | 1:A:154:SER:HB2 | 1:A:166:GLU:HG3 | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1096) | 1:A:154:SER:HB2 | 1:A:166:GLU:HG2 | 1 | 0.14 |
| (1,1096) | 1:A:154:SER:HB2 | 1:A:166:GLU:HG3 | 4 | 0.14 |
| (1,1096) | 1:A:154:SER:HB2 | 1:A:166:GLU:HG2 | 4 | 0.14 |
| (1,1096) | 1:A:154:SER:HB2 | 1:A:166:GLU:HG3 | 7 | 0.14 |
| (1,1096) | 1:A:154:SER:HB2 | 1:A:166:GLU:HG2 | 7 | 0.14 |
| (1,1085) | 1:A:153:VAL:HG11 | 1:A:155:SER:HB3 | 8 | 0.14 |
| (1,1085) | 1:A:153:VAL:HG12 | 1:A:155:SER:HB3 | 8 | 0.14 |
| (1,1085) | 1:A:153:VAL:HG13 | 1:A:155:SER:HB3 | 8 | 0.14 |
| (1,1085) | 1:A:153:VAL:HG21 | 1:A:155:SER:HB3 | 8 | 0.14 |
| (1,1085) | 1:A:153:VAL:HG22 | 1:A:155:SER:HB3 | 8 | 0.14 |
| (1,1085) | 1:A:153:VAL:HG23 | 1:A:155:SER:HB3 | 8 | 0.14 |
| (1,1079) | 1:A:153:VAL:HB | 1:A:154:SER:HA | 3 | 0.14 |
| (1,1065) | 1:A:152:GLN:HB2 | 1:A:169:MET:HA | 2 | 0.14 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 3 | 0.14 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 9 | 0.14 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG21 | 5 | 0.13 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG22 | 5 | 0.13 |
| (1,88) | 1:A:96:ARG:HA | 1:A:165:VAL:HG23 | 5 | 0.13 |
| (1,857) | 1:A:141:LYS:HG2 | 1:A:143:THR:HA | 10 | 0.13 |
| (1,852) | 1:A:141:LYS:HG2 | 1:A:141:LYS:HE2 | 2 | 0.13 |
| (1,852) | 1:A:141:LYS:HG2 | 1:A:141:LYS:HE2 | 9 | 0.13 |
| (1,812) | 1:A:136:ARG:HA | 1:A:136:ARG:HD2 | 3 | 0.13 |
| (1,812) | 1:A:136:ARG:HA | 1:A:136:ARG:HD2 | 4 | 0.13 |
| (1,782) | 1:A:131:HIS:HB2 | 1:A:132:GLY:HA2 | 2 | 0.13 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 1 | 0.13 |
| (1,713) | 1:A:126:GLU:HB2 | 1:A:133:TYR:HB3 | 8 | 0.13 |
| (1,713) | 1:A:126:GLU:HB3 | 1:A:133:TYR:HB3 | 8 | 0.13 |
| (1,71) | 1:A:95:TRP:HB2 | 1:A:168:PRO:HB2 | 6 | 0.13 |
| (1,71) | 1:A:95:TRP:HB3 | 1:A:168:PRO:HB2 | 6 | 0.13 |
| (1,704) | 1:A:125:GLU:HA | 1:A:135:SER:HB3 | 4 | 0.13 |
| (1,684) | 1:A:123:LYS:HA | 1:A:135:SER:HB3 | 8 | 0.13 |
| (1,680) | 1:A:123:LYS:HA | 1:A:123:LYS:HG3 | 1 | 0.13 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG21 | 6 | 0.13 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG22 | 6 | 0.13 |
| (1,68) | 1:A:95:TRP:HB3 | 1:A:148:VAL:HG23 | 6 | 0.13 |
| (1,658) | 1:A:120:ILE:HD11 | 1:A:163:LEU:HA | 1 | 0.13 |
| (1,658) | 1:A:120:ILE:HD12 | 1:A:163:LEU:HA | 1 | 0.13 |
| (1,658) | 1:A:120:ILE:HD13 | 1:A:163:LEU:HA | 1 | 0.13 |
| (1,654) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HD2 | 1 | 0.13 |
| (1,654) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HD2 | 1 | 0.13 |
| (1,654) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HD2 | 1 | 0.13 |
| (1,654) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HD2 | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,654) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HD2 | 4 | 0.13 |
| (1,654) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HD2 | 4 | 0.13 |
| (1,652) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HB2 | 1 | 0.13 |
| (1,652) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HB2 | 1 | 0.13 |
| (1,652) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HB2 | 1 | 0.13 |
| (1,652) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HB2 | 5 | 0.13 |
| (1,652) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HB2 | 5 | 0.13 |
| (1,652) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HB2 | 5 | 0.13 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 4 | 0.13 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 4 | 0.13 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 4 | 0.13 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 4 | 0.13 |
| (1,608) | 1:A:119:GLU:HA | 1:A:141:LYS:HA | 4 | 0.13 |
| (1,605) | 1:A:119:GLU:HA | 1:A:120:ILE:HG13 | 5 | 0.13 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG11 | 4 | 0.13 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG12 | 4 | 0.13 |
| (1,590) | 1:A:118:VAL:HG11 | 1:A:148:VAL:HG13 | 4 | 0.13 |
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG11 | 4 | 0.13 |
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG12 | 4 | 0.13 |
| (1,590) | 1:A:118:VAL:HG12 | 1:A:148:VAL:HG13 | 4 | 0.13 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG11 | 4 | 0.13 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG12 | 4 | 0.13 |
| (1,590) | 1:A:118:VAL:HG13 | 1:A:148:VAL:HG13 | 4 | 0.13 |
| (1,571) | 1:A:118:VAL:HB | 1:A:142:TYR:HD1 | 1 | 0.13 |
| (1,571) | 1:A:118:VAL:HB | 1:A:142:TYR:HD2 | 1 | 0.13 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD21 | 5 | 0.13 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD22 | 5 | 0.13 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD23 | 5 | 0.13 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG21 | 10 | 0.13 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG22 | 10 | 0.13 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG23 | 10 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG11 | 7 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG12 | 7 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG13 | 7 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG21 | 7 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG22 | 7 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG23 | 7 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG11 | 9 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG12 | 9 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG13 | 9 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG21 | 9 | 0.13 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG22 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG23 | 9 | 0.13 |
| (1,479) | 1:A:112:LYS:HE2 | 1:A:121:THR:HG21 | 10 | 0.13 |
| (1,479) | 1:A:112:LYS:HE2 | 1:A:121:THR:HG22 | 10 | 0.13 |
| (1,479) | 1:A:112:LYS:HE2 | 1:A:121:THR:HG23 | 10 | 0.13 |
| (1,479) | 1:A:112:LYS:HE3 | 1:A:121:THR:HG21 | 10 | 0.13 |
| (1,479) | 1:A:112:LYS:HE3 | 1:A:121:THR:HG22 | 10 | 0.13 |
| (1,479) | 1:A:112:LYS:HE3 | 1:A:121:THR:HG23 | 10 | 0.13 |
| (1,465) | 1:A:112:LYS:HG2 | 1:A:118:VAL:HA | 10 | 0.13 |
| (1,465) | 1:A:112:LYS:HG3 | 1:A:118:VAL:HA | 10 | 0.13 |
| (1,4290) | 1:B:171:LYS:H | 1:B:171:LYS:HB2 | 4 | 0.13 |
| (1,4290) | 1:B:171:LYS:H | 1:B:171:LYS:HB3 | 4 | 0.13 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG2 | 10 | 0.13 |
| (1,4264) | 1:B:167:ALA:H | 1:B:166:GLU:HG3 | 10 | 0.13 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD11 | 8 | 0.13 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD12 | 8 | 0.13 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD13 | 8 | 0.13 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD21 | 8 | 0.13 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD22 | 8 | 0.13 |
| (1,4225) | 1:B:164:THR:H | 1:B:163:LEU:HD23 | 8 | 0.13 |
| (1,4220) | 1:B:164:THR:H | 1:B:162:THR:HA | 9 | 0.13 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD11 | 5 | 0.13 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD12 | 5 | 0.13 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD13 | 5 | 0.13 |
| (1,4196) | 1:B:162:THR:H | 1:B:102:ASN:HB2 | 5 | 0.13 |
| (1,419) | 1:A:111:VAL:HA | 1:A:120:ILE:HG13 | 7 | 0.13 |
| (1,418) | 1:A:111:VAL:HA | 1:A:120:ILE:HG12 | 1 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD11 | 7 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD12 | 7 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD13 | 7 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD21 | 7 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD22 | 7 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD23 | 7 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD11 | 8 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD12 | 8 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD13 | 8 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD21 | 8 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD22 | 8 | 0.13 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD23 | 8 | 0.13 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG21 | 2 | 0.13 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG22 | 2 | 0.13 |
| (1,4168) | 1:B:158:SER:H | 1:B:162:THR:HG23 | 2 | 0.13 |
| (1,4160) | 1:B:158:SER:H | 1:B:157:LEU:HG | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD11 | 9 | 0.13 |
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD12 | 9 | 0.13 |
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD13 | 9 | 0.13 |
| (1,413) | 1:A:111:VAL:HA | 1:A:112:LYS:HG2 | 5 | 0.13 |
| (1,413) | 1:A:111:VAL:HA | 1:A:112:LYS:HG3 | 5 | 0.13 |
| (1,4096) | 1:B:153:VAL:H | 1:B:113:THR:HG21 | 2 | 0.13 |
| (1,4096) | 1:B:153:VAL:H | 1:B:113:THR:HG22 | 2 | 0.13 |
| (1,4096) | 1:B:153:VAL:H | 1:B:113:THR:HG23 | 2 | 0.13 |
| (1,4089) | 1:B:152:GLN:HE22 | 1:B:152:GLN:HB2 | 8 | 0.13 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 2 | 0.13 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 2 | 0.13 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 2 | 0.13 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG21 | 8 | 0.13 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG22 | 8 | 0.13 |
| (1,4078) | 1:B:152:GLN:HE21 | 1:B:151:THR:HG23 | 8 | 0.13 |
| (1,4043) | 1:B:149:ASP:H | 1:B:152:GLN:HB2 | 4 | 0.13 |
| (1,4043) | 1:B:149:ASP:H | 1:B:152:GLN:HB2 | 10 | 0.13 |
| (1,4034) | 1:B:148:VAL:H | 1:B:149:ASP:H | 1 | 0.13 |
| (1,3935) | 1:B:134:ILE:H | 1:B:127:ARG:HB2 | 9 | 0.13 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE1 | 4 | 0.13 |
| (1,3932) | 1:B:132:GLY:H | 1:B:133:TYR:HE2 | 4 | 0.13 |
| (1,3928) | 1:B:132:GLY:H | 1:B:131:HIS:HB3 | 7 | 0.13 |
| (1,3928) | 1:B:132:GLY:H | 1:B:131:HIS:HB3 | 8 | 0.13 |
| (1,3881) | 1:B:128:GLN:H | 1:B:127:ARG:HD2 | 8 | 0.13 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD1 | 5 | 0.13 |
| (1,3877) | 1:B:127:ARG:H | 1:B:133:TYR:HD2 | 5 | 0.13 |
| (1,3848) | 1:B:123:LYS:H | 1:B:109:LEU:HG | 3 | 0.13 |
| (1,3834) | 1:B:121:THR:H | 1:B:120:ILE:HG13 | 9 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 1 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 1 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 1 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 1 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 1 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 1 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG21 | 2 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG22 | 2 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG23 | 2 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG11 | 2 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG12 | 2 | 0.13 |
| (1,3831) | 1:B:121:THR:H | 1:B:111:VAL:HG13 | 2 | 0.13 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD11 | 8 | 0.13 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD12 | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD13 | 8 | 0.13 |
| (1,3806) | 1:B:119:GLU:H | 1:B:114:LYS:HB3 | 2 | 0.13 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 4 | 0.13 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 2 | 0.13 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 8 | 0.13 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG11 | 7 | 0.13 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG12 | 7 | 0.13 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG13 | 7 | 0.13 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG21 | 7 | 0.13 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG22 | 7 | 0.13 |
| (1,3787) | 1:B:117:VAL:H | 1:B:118:VAL:HG23 | 7 | 0.13 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG21 | 6 | 0.13 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG22 | 6 | 0.13 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG23 | 6 | 0.13 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG11 | 6 | 0.13 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG12 | 6 | 0.13 |
| (1,3786) | 1:B:117:VAL:H | 1:B:117:VAL:HG13 | 6 | 0.13 |
| (1,3770) | 1:B:114:LYS:H | 1:B:119:GLU:H | 6 | 0.13 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 5 | 0.13 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 3 | 0.13 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 3 | 0.13 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 3 | 0.13 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 3 | 0.13 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 3 | 0.13 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 3 | 0.13 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 5 | 0.13 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 5 | 0.13 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 5 | 0.13 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 5 | 0.13 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 5 | 0.13 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 5 | 0.13 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD21 | 9 | 0.13 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD22 | 9 | 0.13 |
| (1,361) | 1:A:109:LEU:HB3 | 1:A:109:LEU:HD23 | 9 | 0.13 |
| (1,3608) | 1:B:94:ARG:H | 1:B:169:MET:HG2 | 9 | 0.13 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 10 | 0.13 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 7 | 0.13 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD2 | 10 | 0.13 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD2 | 10 | 0.13 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD3 | 10 | 0.13 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD3 | 10 | 0.13 |
| (1,3479) | 1:B:159:PRO:HA | 1:B:159:PRO:HB3 | 7 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3474) | 1:B:158:SER:HB3 | 1:B:160:GLU:HB3 | 4 | 0.13 |
| (1,3474) | 1:B:158:SER:HB3 | 1:B:160:GLU:HB3 | 10 | 0.13 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD3 | 1 | 0.13 |
| (1,347) | 1:A:108:GLU:HG3 | 1:A:123:LYS:HD2 | 1 | 0.13 |
| (1,3454) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HB3 | 6 | 0.13 |
| (1,3454) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HB3 | 6 | 0.13 |
| (1,3454) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HB3 | 6 | 0.13 |
| (1,345) | 1:A:108:GLU:HG2 | 1:A:123:LYS:HE3 | 7 | 0.13 |
| (1,345) | 1:A:108:GLU:HG2 | 1:A:123:LYS:HE2 | 7 | 0.13 |
| (1,3438) | 1:B:157:LEU:HB3 | 1:B:157:LEU:HG | 1 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD11 | 10 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD12 | 10 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD13 | 10 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD21 | 10 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD22 | 10 | 0.13 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD23 | 10 | 0.13 |
| (1,3385) | 1:B:155:SER:HA | 1:B:156:SER:HB3 | 3 | 0.13 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG3 | 1 | 0.13 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG2 | 1 | 0.13 |
| (1,3367) | 1:B:153:VAL:HG11 | 1:B:165:VAL:HA | 8 | 0.13 |
| (1,3367) | 1:B:153:VAL:HG12 | 1:B:165:VAL:HA | 8 | 0.13 |
| (1,3367) | 1:B:153:VAL:HG13 | 1:B:165:VAL:HA | 8 | 0.13 |
| (1,3367) | 1:B:153:VAL:HG21 | 1:B:165:VAL:HA | 8 | 0.13 |
| (1,3367) | 1:B:153:VAL:HG22 | 1:B:165:VAL:HA | 8 | 0.13 |
| (1,3367) | 1:B:153:VAL:HG23 | 1:B:165:VAL:HA | 8 | 0.13 |
| (1,3360) | 1:B:153:VAL:HB | 1:B:154:SER:HA | 5 | 0.13 |
| (1,3358) | 1:B:153:VAL:HA | 1:B:168:PRO:HD2 | 7 | 0.13 |
| (1,331) | 1:A:107:ASP:HA | 1:A:108:GLU:HG2 | 7 | 0.13 |
| (1,33) | 1:A:94:ARG:HA | 1:A:169:MET:HB2 | 9 | 0.13 |
| (1,3288) | 1:B:148:VAL:HG11 | 1:B:153:VAL:HA | 7 | 0.13 |
| (1,3288) | 1:B:148:VAL:HG12 | 1:B:153:VAL:HA | 7 | 0.13 |
| (1,3288) | 1:B:148:VAL:HG13 | 1:B:153:VAL:HA | 7 | 0.13 |
| (1,3288) | 1:B:148:VAL:HG11 | 1:B:153:VAL:HA | 10 | 0.13 |
| (1,3288) | 1:B:148:VAL:HG12 | 1:B:153:VAL:HA | 10 | 0.13 |
| (1,3288) | 1:B:148:VAL:HG13 | 1:B:153:VAL:HA | 10 | 0.13 |
| (1,3258) | 1:B:147:GLY:HA3 | 1:B:148:VAL:HB | 9 | 0.13 |
| (1,3249) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA3 | 7 | 0.13 |
| (1,3239) | 1:B:145:PRO:HG3 | 1:B:146:PRO:HD2 | 5 | 0.13 |
| (1,32) | 1:A:94:ARG:HA | 1:A:168:PRO:HD3 | 2 | 0.13 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 10 | 0.13 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 10 | 0.13 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 3 | 0.13 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 3 | 0.13 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 3 | 0.13 |
| (1,3163) | 1:B:142:TYR:HD1 | 1:B:165:VAL:HG11 | 2 | 0.13 |
| (1,3163) | 1:B:142:TYR:HD1 | 1:B:165:VAL:HG12 | 2 | 0.13 |
| (1,3163) | 1:B:142:TYR:HD1 | 1:B:165:VAL:HG13 | 2 | 0.13 |
| (1,3163) | 1:B:142:TYR:HD2 | 1:B:165:VAL:HG11 | 2 | 0.13 |
| (1,3163) | 1:B:142:TYR:HD2 | 1:B:165:VAL:HG12 | 2 | 0.13 |
| (1,3163) | 1:B:142:TYR:HD2 | 1:B:165:VAL:HG13 | 2 | 0.13 |
| (1,3153) | 1:B:142:TYR:HB2 | 1:B:143:THR:HB | 5 | 0.13 |
| (1,3143) | 1:B:141:LYS:HG3 | 1:B:142:TYR:HB3 | 5 | 0.13 |
| (1,3133) | 1:B:141:LYS:HG2 | 1:B:141:LYS:HE2 | 2 | 0.13 |
| (1,3093) | 1:B:136:ARG:HA | 1:B:136:ARG:HD2 | 10 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD1 | 3 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD2 | 3 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD1 | 3 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD2 | 3 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD1 | 3 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD2 | 3 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD1 | 10 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG21 | 1:B:133:TYR:HD2 | 10 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD1 | 10 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG22 | 1:B:133:TYR:HD2 | 10 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD1 | 10 | 0.13 |
| (1,3078) | 1:B:134:ILE:HG23 | 1:B:133:TYR:HD2 | 10 | 0.13 |
| (1,3048) | 1:B:129:ASP:HA | 1:B:133:TYR:HA | 4 | 0.13 |
| (1,3037) | 1:B:128:GLN:HB3 | 1:B:133:TYR:HD1 | 9 | 0.13 |
| (1,3037) | 1:B:128:GLN:HB3 | 1:B:133:TYR:HD2 | 9 | 0.13 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE1 | 5 | 0.13 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE2 | 5 | 0.13 |
| (1,3015) | 1:B:127:ARG:HA | 1:B:127:ARG:HB3 | 1 | 0.13 |
| (1,3015) | 1:B:127:ARG:HA | 1:B:127:ARG:HB3 | 9 | 0.13 |
| (1,2994) | 1:B:126:GLU:HB2 | 1:B:133:TYR:HB3 | 6 | 0.13 |
| (1,2994) | 1:B:126:GLU:HB3 | 1:B:133:TYR:HB3 | 6 | 0.13 |
| (1,2985) | 1:B:125:GLU:HA | 1:B:135:SER:HB3 | 2 | 0.13 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 10 | 0.13 |
| (1,2933) | 1:B:120:ILE:HD11 | 1:B:140:ARG:HB2 | 4 | 0.13 |
| (1,2933) | 1:B:120:ILE:HD12 | 1:B:140:ARG:HB2 | 4 | 0.13 |
| (1,2933) | 1:B:120:ILE:HD13 | 1:B:140:ARG:HB2 | 4 | 0.13 |
| (1,2928) | 1:B:120:ILE:HG21 | 1:B:122:GLY:HA3 | 7 | 0.13 |
| (1,2928) | 1:B:120:ILE:HG22 | 1:B:122:GLY:HA3 | 7 | 0.13 |
| (1,2928) | 1:B:120:ILE:HG23 | 1:B:122:GLY:HA3 | 7 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 5 | 0.13 |
| (1,2885) | 1:B:119:GLU:HA | 1:B:120:ILE:HG12 | 5 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 7 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 7 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 7 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 7 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 7 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 7 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 7 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 7 | 0.13 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 7 | 0.13 |
| (1,2866) | 1:B:118:VAL:HG11 | 1:B:142:TYR:HD1 | 9 | 0.13 |
| (1,2866) | 1:B:118:VAL:HG11 | 1:B:142:TYR:HD2 | 9 | 0.13 |
| (1,2866) | 1:B:118:VAL:HG12 | 1:B:142:TYR:HD1 | 9 | 0.13 |
| (1,2866) | 1:B:118:VAL:HG12 | 1:B:142:TYR:HD2 | 9 | 0.13 |
| (1,2866) | 1:B:118:VAL:HG13 | 1:B:142:TYR:HD1 | 9 | 0.13 |
| (1,2866) | 1:B:118:VAL:HG13 | 1:B:142:TYR:HD2 | 9 | 0.13 |
| (1,2858) | 1:B:118:VAL:HB | 1:B:153:VAL:HG21 | 5 | 0.13 |
| (1,2858) | 1:B:118:VAL:HB | 1:B:153:VAL:HG22 | 5 | 0.13 |
| (1,2858) | 1:B:118:VAL:HB | 1:B:153:VAL:HG23 | 5 | 0.13 |
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD21 | 9 | 0.13 |
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD22 | 9 | 0.13 |
| (1,2847) | 1:B:118:VAL:HA | 1:B:144:LEU:HD23 | 9 | 0.13 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG21 | 6 | 0.13 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG22 | 6 | 0.13 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG23 | 6 | 0.13 |
| (1,2798) | 1:B:115:ASP:HB3 | 1:B:150:PRO:HG2 | 2 | 0.13 |
| (1,279) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA2 | 3 | 0.13 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG11 | 2 | 0.13 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG12 | 2 | 0.13 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG13 | 2 | 0.13 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG21 | 2 | 0.13 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG22 | 2 | 0.13 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG23 | 2 | 0.13 |
| (1,2760) | 1:B:112:LYS:HE2 | 1:B:121:THR:HG21 | 5 | 0.13 |
| (1,2760) | 1:B:112:LYS:HE2 | 1:B:121:THR:HG22 | 5 | 0.13 |
| (1,2760) | 1:B:112:LYS:HE2 | 1:B:121:THR:HG23 | 5 | 0.13 |
| (1,2760) | 1:B:112:LYS:HE3 | 1:B:121:THR:HG21 | 5 | 0.13 |
| (1,2760) | 1:B:112:LYS:HE3 | 1:B:121:THR:HG22 | 5 | 0.13 |
| (1,2760) | 1:B:112:LYS:HE3 | 1:B:121:THR:HG23 | 5 | 0.13 |
| (1,2746) | 1:B:112:LYS:HG2 | 1:B:118:VAL:HA | 2 | 0.13 |
| (1,2746) | 1:B:112:LYS:HG3 | 1:B:118:VAL:HA | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2738) | 1:B:112:LYS:HB2 | 1:B:120:ILE:HA | 4 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG21 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG22 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG23 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG21 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG22 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG23 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG21 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG22 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG23 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG21 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG22 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG23 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG21 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG22 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG23 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG21 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG22 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG23 | 5 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG21 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG22 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG11 | 1:B:118:VAL:HG23 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG21 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG22 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG12 | 1:B:118:VAL:HG23 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG21 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG22 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG13 | 1:B:118:VAL:HG23 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG21 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG22 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG21 | 1:B:118:VAL:HG23 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG21 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG22 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG22 | 1:B:118:VAL:HG23 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG21 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG22 | 6 | 0.13 |
| (1,2713) | 1:B:111:VAL:HG23 | 1:B:118:VAL:HG23 | 6 | 0.13 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD11 | 7 | 0.13 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD12 | 7 | 0.13 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD13 | 7 | 0.13 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD21 | 7 | 0.13 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD22 | 7 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD23 | 7 | 0.13 |
| (1,2702) | 1:B:111:VAL:HA | 1:B:163:LEU:HD11 | 5 | 0.13 |
| (1,2702) | 1:B:111:VAL:HA | 1:B:163:LEU:HD12 | 5 | 0.13 |
| (1,2702) | 1:B:111:VAL:HA | 1:B:163:LEU:HD13 | 5 | 0.13 |
| (1,2702) | 1:B:111:VAL:HA | 1:B:163:LEU:HD21 | 5 | 0.13 |
| (1,2702) | 1:B:111:VAL:HA | 1:B:163:LEU:HD22 | 5 | 0.13 |
| (1,2702) | 1:B:111:VAL:HA | 1:B:163:LEU:HD23 | 5 | 0.13 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 1 | 0.13 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 10 | 0.13 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 1 | 0.13 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 1 | 0.13 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 1 | 0.13 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD11 | 3 | 0.13 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD12 | 3 | 0.13 |
| (1,269) | 1:A:101:VAL:HB | 1:A:157:LEU:HD13 | 3 | 0.13 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG2 | 7 | 0.13 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG3 | 7 | 0.13 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 8 | 0.13 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 8 | 0.13 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 8 | 0.13 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 8 | 0.13 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 8 | 0.13 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 8 | 0.13 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD21 | 8 | 0.13 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD22 | 8 | 0.13 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD23 | 8 | 0.13 |
| (1,2640) | 1:B:109:LEU:HB2 | 1:B:122:GLY:HA2 | 4 | 0.13 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD11 | 7 | 0.13 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD12 | 7 | 0.13 |
| (1,2639) | 1:B:109:LEU:HB2 | 1:B:109:LEU:HD13 | 7 | 0.13 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG21 | 3 | 0.13 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG22 | 3 | 0.13 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG23 | 3 | 0.13 |
| (1,2613) | 1:B:107:ASP:HA | 1:B:108:GLU:HG3 | 1 | 0.13 |
| (1,259) | 1:A:100:ASP:HA | 1:A:100:ASP:HB3 | 2 | 0.13 |
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD11 | 7 | 0.13 |
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD12 | 7 | 0.13 |
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD13 | 7 | 0.13 |
| (1,2564) | 1:B:105:ALA:HA | 1:B:106:PRO:HB3 | 7 | 0.13 |
| (1,2559) | 1:B:102:ASN:HB2 | 1:B:161:GLY:HA3 | 4 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG21 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG22 | 1 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG23 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG21 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG22 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG23 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG21 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG22 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG23 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG11 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG12 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG13 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG11 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG12 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG13 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG11 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG12 | 1 | 0.13 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG13 | 1 | 0.13 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD1 | 8 | 0.13 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD2 | 8 | 0.13 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD1 | 8 | 0.13 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD2 | 8 | 0.13 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD1 | 8 | 0.13 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD2 | 8 | 0.13 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG21 | 10 | 0.13 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG22 | 10 | 0.13 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG23 | 10 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 2 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 2 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 2 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 3 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 3 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 3 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG11 | 10 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG12 | 10 | 0.13 |
| (1,2410) | 1:B:97:VAL:HB | 1:B:148:VAL:HG13 | 10 | 0.13 |
| (1,2400) | 1:B:97:VAL:HA | 1:B:97:VAL:HG11 | 10 | 0.13 |
| (1,2400) | 1:B:97:VAL:HA | 1:B:97:VAL:HG12 | 10 | 0.13 |
| (1,2400) | 1:B:97:VAL:HA | 1:B:97:VAL:HG13 | 10 | 0.13 |
| (1,2382) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HA | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD21 | 1:A:101:VAL:HG21 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD21 | 1:A:101:VAL:HG22 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD21 | 1:A:101:VAL:HG23 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD22 | 1:A:101:VAL:HG21 | 6 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,238) | 1:A:99:LEU:HD22 | 1:A:101:VAL:HG22 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD22 | 1:A:101:VAL:HG23 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD23 | 1:A:101:VAL:HG21 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD23 | 1:A:101:VAL:HG22 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD23 | 1:A:101:VAL:HG23 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD21 | 1:A:101:VAL:HG11 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD21 | 1:A:101:VAL:HG12 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD21 | 1:A:101:VAL:HG13 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD22 | 1:A:101:VAL:HG11 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD22 | 1:A:101:VAL:HG12 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD22 | 1:A:101:VAL:HG13 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD23 | 1:A:101:VAL:HG11 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD23 | 1:A:101:VAL:HG12 | 6 | 0.13 |
| (1,238) | 1:A:99:LEU:HD23 | 1:A:101:VAL:HG13 | 6 | 0.13 |
| (1,236) | 1:A:99:LEU:HD11 | 1:A:164:THR:HA | 4 | 0.13 |
| (1,236) | 1:A:99:LEU:HD12 | 1:A:164:THR:HA | 4 | 0.13 |
| (1,236) | 1:A:99:LEU:HD13 | 1:A:164:THR:HA | 4 | 0.13 |
| (1,2357) | 1:B:95:TRP:HE3 | 1:B:166:GLU:HA | 8 | 0.13 |
| (1,2352) | 1:B:95:TRP:HB2 | 1:B:168:PRO:HB2 | 7 | 0.13 |
| (1,2352) | 1:B:95:TRP:HB3 | 1:B:168:PRO:HB2 | 7 | 0.13 |
| (1,2352) | 1:B:95:TRP:HB2 | 1:B:168:PRO:HB2 | 9 | 0.13 |
| (1,2352) | 1:B:95:TRP:HB3 | 1:B:168:PRO:HB2 | 9 | 0.13 |
| (1,2352) | 1:B:95:TRP:HB2 | 1:B:168:PRO:HB2 | 10 | 0.13 |
| (1,2352) | 1:B:95:TRP:HB3 | 1:B:168:PRO:HB2 | 10 | 0.13 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG21 | 2 | 0.13 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG22 | 2 | 0.13 |
| (1,2349) | 1:B:95:TRP:HB3 | 1:B:148:VAL:HG23 | 2 | 0.13 |
| (1,2329) | 1:B:94:ARG:HD2 | 1:B:168:PRO:HA | 4 | 0.13 |
| (1,2315) | 1:B:94:ARG:HB2 | 1:B:94:ARG:HG2 | 9 | 0.13 |
| (1,2304) | 1:B:94:ARG:HA | 1:B:94:ARG:HB3 | 8 | 0.13 |
| (1,23) | 1:A:94:ARG:HA | 1:A:94:ARG:HB3 | 3 | 0.13 |
| (1,23) | 1:A:94:ARG:HA | 1:A:94:ARG:HB3 | 4 | 0.13 |
| (1,23) | 1:A:94:ARG:HA | 1:A:94:ARG:HB3 | 10 | 0.13 |
| (1,2296) | 1:B:93:ASP:HA | 1:B:94:ARG:HB2 | 5 | 0.13 |
| (1,2296) | 1:B:93:ASP:HA | 1:B:94:ARG:HB3 | 5 | 0.13 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB1 | 8 | 0.13 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB2 | 8 | 0.13 |
| (1,2292) | 1:B:91:THR:HB | 1:B:92:ALA:HB3 | 8 | 0.13 |
| (1,2225) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 5 | 0.13 |
| (1,2225) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 5 | 0.13 |
| (1,2225) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 5 | 0.13 |
| (1,2093) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2093) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 5 | 0.13 |
| (1,2093) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 5 | 0.13 |
| (1,2000) | 1:A:169:MET:H | 1:A:169:MET:HG3 | 5 | 0.13 |
| (1,1981) | 1:A:167:ALA:H | 1:A:166:GLU:HB2 | 3 | 0.13 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD11 | 5 | 0.13 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD12 | 5 | 0.13 |
| (1,1938) | 1:A:164:THR:H | 1:A:157:LEU:HD13 | 5 | 0.13 |
| (1,1935) | 1:A:163:LEU:H | 1:A:164:THR:H | 2 | 0.13 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 3 | 0.13 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 9 | 0.13 |
| (1,1902) | 1:A:161:GLY:H | 1:A:102:ASN:HB3 | 8 | 0.13 |
| (1,1901) | 1:A:161:GLY:H | 1:A:102:ASN:HB2 | 1 | 0.13 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD11 | 6 | 0.13 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD12 | 6 | 0.13 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD13 | 6 | 0.13 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD21 | 6 | 0.13 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD22 | 6 | 0.13 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD23 | 6 | 0.13 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG21 | 7 | 0.13 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG22 | 7 | 0.13 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG23 | 7 | 0.13 |
| (1,187) | 1:A:98:SER:HB2 | 1:A:164:THR:HB | 3 | 0.13 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG11 | 10 | 0.13 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG12 | 10 | 0.13 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG13 | 10 | 0.13 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG21 | 10 | 0.13 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG22 | 10 | 0.13 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG23 | 10 | 0.13 |
| (1,1849) | 1:A:155:SER:H | 1:A:156:SER:HA | 7 | 0.13 |
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 2 | 0.13 |
| (1,1796) | 1:A:152:GLN:HE21 | 1:A:149:ASP:HB2 | 7 | 0.13 |
| (1,1766) | 1:A:149:ASP:H | 1:A:169:MET:HG3 | 3 | 0.13 |
| (1,176) | 1:A:98:SER:HA | 1:A:162:THR:HG21 | 3 | 0.13 |
| (1,176) | 1:A:98:SER:HA | 1:A:162:THR:HG22 | 3 | 0.13 |
| (1,176) | 1:A:98:SER:HA | 1:A:162:THR:HG23 | 3 | 0.13 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD2 | 2 | 0.13 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD3 | 2 | 0.13 |
| (1,1751) | 1:A:148:VAL:H | 1:A:149:ASP:HA | 6 | 0.13 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 10 | 0.13 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 10 | 0.13 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 10 | 0.13 |
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG21 | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG22 | 2 | 0.13 |
| (1,1669) | 1:A:136:ARG:H | 1:A:134:ILE:HG23 | 2 | 0.13 |
| (1,1654) | 1:A:134:ILE:H | 1:A:127:ARG:HB2 | 8 | 0.13 |
| (1,1627) | 1:A:129:ASP:H | 1:A:132:GLY:H | 3 | 0.13 |
| (1,1617) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HG3 | 6 | 0.13 |
| (1,1588) | 1:A:126:GLU:H | 1:A:125:GLU:HG3 | 1 | 0.13 |
| (1,1588) | 1:A:126:GLU:H | 1:A:125:GLU:HG3 | 9 | 0.13 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD11 | 8 | 0.13 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD12 | 8 | 0.13 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD13 | 8 | 0.13 |
| (1,1525) | 1:A:119:GLU:H | 1:A:114:LYS:HB3 | 7 | 0.13 |
| (1,1467) | 1:A:113:THR:H | 1:A:112:LYS:HB2 | 3 | 0.13 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB2 | 2 | 0.13 |
| (1,1462) | 1:A:112:LYS:H | 1:A:119:GLU:HB3 | 2 | 0.13 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD11 | 2 | 0.13 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD12 | 2 | 0.13 |
| (1,1449) | 1:A:111:VAL:H | 1:A:120:ILE:HD13 | 2 | 0.13 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD1 | 6 | 0.13 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD2 | 6 | 0.13 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD1 | 6 | 0.13 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD2 | 6 | 0.13 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD1 | 6 | 0.13 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD2 | 6 | 0.13 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD21 | 3 | 0.13 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD22 | 3 | 0.13 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD23 | 3 | 0.13 |
| (1,1373) | 1:A:102:ASN:HD21 | 1:A:161:GLY:HA2 | 4 | 0.13 |
| (1,1362) | 1:A:101:VAL:H | 1:A:120:ILE:HG21 | 1 | 0.13 |
| (1,1362) | 1:A:101:VAL:H | 1:A:120:ILE:HG22 | 1 | 0.13 |
| (1,1362) | 1:A:101:VAL:H | 1:A:120:ILE:HG23 | 1 | 0.13 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 7 | 0.13 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 7 | 0.13 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 7 | 0.13 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 7 | 0.13 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 7 | 0.13 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 7 | 0.13 |
| (1,1345) | 1:A:97:VAL:H | 1:A:165:VAL:H | 3 | 0.13 |
| (1,1328) | 1:A:94:ARG:H | 1:A:169:MET:HG3 | 8 | 0.13 |
| (1,1311) | 1:A:170:PRO:HB2 | 1:A:170:PRO:HG2 | 9 | 0.13 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 9 | 0.13 |
| (1,1285) | 1:A:168:PRO:HD2 | 1:A:169:MET:HA | 5 | 0.13 |
| (1,1258) | 1:A:166:GLU:HG2 | 1:A:167:ALA:HA | 6 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1258) | 1:A:166:GLU:HG3 | 1:A:167:ALA:HA | 6 | 0.13 |
| (1,1217) | 1:A:161:GLY:HA3 | 1:A:163:LEU:HA | 5 | 0.13 |
| (1,1174) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HG | 8 | 0.13 |
| (1,1174) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HG | 8 | 0.13 |
| (1,1174) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HG | 8 | 0.13 |
| (1,1172) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB2 | 7 | 0.13 |
| (1,1172) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB2 | 7 | 0.13 |
| (1,1172) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB2 | 7 | 0.13 |
| (1,1168) | 1:A:157:LEU:HD11 | 1:A:161:GLY:HA3 | 6 | 0.13 |
| (1,1168) | 1:A:157:LEU:HD12 | 1:A:161:GLY:HA3 | 6 | 0.13 |
| (1,1168) | 1:A:157:LEU:HD13 | 1:A:161:GLY:HA3 | 6 | 0.13 |
| (1,1157) | 1:A:157:LEU:HB3 | 1:A:157:LEU:HG | 5 | 0.13 |
| (1,1157) | 1:A:157:LEU:HB3 | 1:A:157:LEU:HG | 7 | 0.13 |
| (1,1157) | 1:A:157:LEU:HB3 | 1:A:157:LEU:HG | 9 | 0.13 |
| (1,1149) | 1:A:157:LEU:HA | 1:A:163:LEU:HB3 | 3 | 0.13 |
| (1,1110) | 1:A:155:SER:HA | 1:A:165:VAL:HA | 2 | 0.13 |
| (1,1110) | 1:A:155:SER:HA | 1:A:165:VAL:HA | 8 | 0.13 |
| (1,1079) | 1:A:153:VAL:HB | 1:A:154:SER:HA | 6 | 0.13 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG3 | 8 | 0.13 |
| (1,107) | 1:A:96:ARG:HG2 | 1:A:166:GLU:HG2 | 8 | 0.13 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 7 | 0.13 |
| (1,1028) | 1:A:149:ASP:HA | 1:A:150:PRO:HD3 | 8 | 0.13 |
| (1,1020) | 1:A:148:VAL:HG21 | 1:A:169:MET:HB2 | 4 | 0.13 |
| (1,1020) | 1:A:148:VAL:HG22 | 1:A:169:MET:HB2 | 4 | 0.13 |
| (1,1020) | 1:A:148:VAL:HG23 | 1:A:169:MET:HB2 | 4 | 0.13 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 4 | 0.12 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 4 | 0.12 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 4 | 0.12 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG11 | 4 | 0.12 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG12 | 4 | 0.12 |
| (1,912) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG13 | 4 | 0.12 |
| (1,849) | 1:A:141:LYS:HB2 | 1:A:141:LYS:HE2 | 7 | 0.12 |
| (1,805) | 1:A:134:ILE:HG21 | 1:A:135:SER:HB2 | 7 | 0.12 |
| (1,805) | 1:A:134:ILE:HG22 | 1:A:135:SER:HB2 | 7 | 0.12 |
| (1,805) | 1:A:134:ILE:HG23 | 1:A:135:SER:HB2 | 7 | 0.12 |
| (1,805) | 1:A:134:ILE:HD11 | 1:A:135:SER:HB2 | 7 | 0.12 |
| (1,805) | 1:A:134:ILE:HD12 | 1:A:135:SER:HB2 | 7 | 0.12 |
| (1,805) | 1:A:134:ILE:HD13 | 1:A:135:SER:HB2 | 7 | 0.12 |
| (1,782) | 1:A:131:HIS:HB2 | 1:A:132:GLY:HA2 | 10 | 0.12 |
| (1,764) | 1:A:129:ASP:HA | 1:A:129:ASP:HB3 | 4 | 0.12 |
| (1,719) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HD1 | 10 | 0.12 |
| (1,719) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HD2 | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,718) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HB3 | 9 | 0.12 |
| (1,713) | 1:A:126:GLU:HB2 | 1:A:133:TYR:HB3 | 5 | 0.12 |
| (1,713) | 1:A:126:GLU:HB3 | 1:A:133:TYR:HB3 | 5 | 0.12 |
| (1,680) | 1:A:123:LYS:HA | 1:A:123:LYS:HG3 | 5 | 0.12 |
| (1,652) | 1:A:120:ILE:HD11 | 1:A:140:ARG:HB2 | 2 | 0.12 |
| (1,652) | 1:A:120:ILE:HD12 | 1:A:140:ARG:HB2 | 2 | 0.12 |
| (1,652) | 1:A:120:ILE:HD13 | 1:A:140:ARG:HB2 | 2 | 0.12 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 7 | 0.12 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 7 | 0.12 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 7 | 0.12 |
| (1,608) | 1:A:119:GLU:HA | 1:A:141:LYS:HA | 5 | 0.12 |
| (1,577) | 1:A:118:VAL:HB | 1:A:153:VAL:HG21 | 4 | 0.12 |
| (1,577) | 1:A:118:VAL:HB | 1:A:153:VAL:HG22 | 4 | 0.12 |
| (1,577) | 1:A:118:VAL:HB | 1:A:153:VAL:HG23 | 4 | 0.12 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD21 | 3 | 0.12 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD22 | 3 | 0.12 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD23 | 3 | 0.12 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 2 | 0.12 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 2 | 0.12 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 2 | 0.12 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG21 | 1 | 0.12 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG22 | 1 | 0.12 |
| (1,546) | 1:A:117:VAL:HA | 1:A:143:THR:HG23 | 1 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 1 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 1 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 1 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 4 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 4 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 4 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG21 | 7 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG22 | 7 | 0.12 |
| (1,521) | 1:A:116:GLY:HA2 | 1:A:118:VAL:HG23 | 7 | 0.12 |
| (1,517) | 1:A:115:ASP:HB3 | 1:A:150:PRO:HG2 | 9 | 0.12 |
| (1,513) | 1:A:115:ASP:HB2 | 1:A:117:VAL:HG21 | 6 | 0.12 |
| (1,513) | 1:A:115:ASP:HB2 | 1:A:117:VAL:HG22 | 6 | 0.12 |
| (1,513) | 1:A:115:ASP:HB2 | 1:A:117:VAL:HG23 | 6 | 0.12 |
| (1,513) | 1:A:115:ASP:HB2 | 1:A:117:VAL:HG11 | 6 | 0.12 |
| (1,513) | 1:A:115:ASP:HB2 | 1:A:117:VAL:HG12 | 6 | 0.12 |
| (1,513) | 1:A:115:ASP:HB2 | 1:A:117:VAL:HG13 | 6 | 0.12 |
| (1,509) | 1:A:114:LYS:HA | 1:A:114:LYS:HB2 | 6 | 0.12 |
| (1,502) | 1:A:113:THR:HG21 | 1:A:150:PRO:HB3 | 2 | 0.12 |
| (1,502) | 1:A:113:THR:HG22 | 1:A:150:PRO:HB3 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,502) | 1:A:113:THR:HG23 | 1:A:150:PRO:HB3 | 2 | 0.12 |
| (1,502) | 1:A:113:THR:HG21 | 1:A:150:PRO:HB3 | 9 | 0.12 |
| (1,502) | 1:A:113:THR:HG22 | 1:A:150:PRO:HB3 | 9 | 0.12 |
| (1,502) | 1:A:113:THR:HG23 | 1:A:150:PRO:HB3 | 9 | 0.12 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG11 | 3 | 0.12 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG12 | 3 | 0.12 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG13 | 3 | 0.12 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG21 | 3 | 0.12 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG22 | 3 | 0.12 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG23 | 3 | 0.12 |
| (1,470) | 1:A:112:LYS:HD2 | 1:A:113:THR:HA | 4 | 0.12 |
| (1,470) | 1:A:112:LYS:HD3 | 1:A:113:THR:HA | 4 | 0.12 |
| (1,465) | 1:A:112:LYS:HG2 | 1:A:118:VAL:HA | 2 | 0.12 |
| (1,465) | 1:A:112:LYS:HG3 | 1:A:118:VAL:HA | 2 | 0.12 |
| (1,465) | 1:A:112:LYS:HG2 | 1:A:118:VAL:HA | 8 | 0.12 |
| (1,465) | 1:A:112:LYS:HG3 | 1:A:118:VAL:HA | 8 | 0.12 |
| (1,4263) | 1:B:167:ALA:H | 1:B:166:GLU:HB3 | 3 | 0.12 |
| (1,4263) | 1:B:167:ALA:H | 1:B:166:GLU:HB3 | 9 | 0.12 |
| (1,4262) | 1:B:167:ALA:H | 1:B:166:GLU:HB2 | 7 | 0.12 |
| (1,4239) | 1:B:165:VAL:H | 1:B:166:GLU:HB3 | 7 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD11 | 4 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD12 | 4 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD13 | 4 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD11 | 7 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD12 | 7 | 0.12 |
| (1,4219) | 1:B:164:THR:H | 1:B:157:LEU:HD13 | 7 | 0.12 |
| (1,4216) | 1:B:163:LEU:H | 1:B:164:THR:H | 9 | 0.12 |
| (1,4213) | 1:B:163:LEU:H | 1:B:100:ASP:HB2 | 5 | 0.12 |
| (1,4213) | 1:B:163:LEU:H | 1:B:100:ASP:HB3 | 5 | 0.12 |
| (1,4190) | 1:B:161:GLY:H | 1:B:160:GLU:HB3 | 5 | 0.12 |
| (1,419) | 1:A:111:VAL:HA | 1:A:120:ILE:HG13 | 6 | 0.12 |
| (1,4183) | 1:B:161:GLY:H | 1:B:102:ASN:HB3 | 6 | 0.12 |
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD11 | 1 | 0.12 |
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD12 | 1 | 0.12 |
| (1,4158) | 1:B:158:SER:H | 1:B:109:LEU:HD13 | 1 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG11 | 1 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG12 | 1 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG13 | 1 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG21 | 1 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG22 | 1 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG23 | 1 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG11 | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG12 | 5 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG13 | 5 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG21 | 5 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG22 | 5 | 0.12 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG23 | 5 | 0.12 |
| (1,4135) | 1:B:155:SER:H | 1:B:166:GLU:HG2 | 5 | 0.12 |
| (1,4135) | 1:B:155:SER:H | 1:B:166:GLU:HG3 | 5 | 0.12 |
| (1,4135) | 1:B:155:SER:H | 1:B:166:GLU:HG2 | 8 | 0.12 |
| (1,4135) | 1:B:155:SER:H | 1:B:166:GLU:HG3 | 8 | 0.12 |
| (1,4086) | 1:B:152:GLN:HE21 | 1:B:170:PRO:HD2 | 3 | 0.12 |
| (1,4086) | 1:B:152:GLN:HE21 | 1:B:170:PRO:HD3 | 3 | 0.12 |
| (1,4047) | 1:B:149:ASP:H | 1:B:169:MET:HG3 | 6 | 0.12 |
| (1,4032) | 1:B:148:VAL:H | 1:B:149:ASP:HA | 5 | 0.12 |
| (1,3955) | 1:B:137:CYS:H | 1:B:136:ARG:HB3 | 5 | 0.12 |
| (1,3948) | 1:B:135:SER:H | 1:B:135:SER:HB2 | 4 | 0.12 |
| (1,3928) | 1:B:132:GLY:H | 1:B:131:HIS:HB3 | 9 | 0.12 |
| (1,3923) | 1:B:132:GLY:H | 1:B:129:ASP:HB2 | 6 | 0.12 |
| (1,3918) | 1:B:131:HIS:H | 1:B:130:GLU:HG2 | 3 | 0.12 |
| (1,3918) | 1:B:131:HIS:H | 1:B:130:GLU:HG3 | 3 | 0.12 |
| (1,3903) | 1:B:129:ASP:H | 1:B:129:ASP:HB3 | 5 | 0.12 |
| (1,3860) | 1:B:124:HIS:H | 1:B:138:PHE:HD1 | 2 | 0.12 |
| (1,3860) | 1:B:124:HIS:H | 1:B:138:PHE:HD2 | 2 | 0.12 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD21 | 1 | 0.12 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD22 | 1 | 0.12 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD23 | 1 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG21 | 7 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG22 | 7 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG23 | 7 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG21 | 8 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG22 | 8 | 0.12 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG23 | 8 | 0.12 |
| (1,3798) | 1:B:118:VAL:H | 1:B:142:TYR:HB2 | 2 | 0.12 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 6 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG21 | 9 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG22 | 9 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG23 | 9 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG11 | 9 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG12 | 9 | 0.12 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG13 | 9 | 0.12 |
| (1,3723) | 1:B:110:THR:H | 1:B:122:GLY:H | 9 | 0.12 |
| (1,3720) | 1:B:110:THR:H | 1:B:120:ILE:HD11 | 9 | 0.12 |
| (1,3720) | 1:B:110:THR:H | 1:B:120:ILE:HD12 | 9 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3720) | 1:B:110:THR:H | 1:B:120:ILE:HD13 | 9 | 0.12 |
| (1,3692) | 1:B:108:GLU:H | 1:B:105:ALA:HA | 2 | 0.12 |
| (1,3670) | 1:B:105:ALA:H | 1:B:106:PRO:HD3 | 7 | 0.12 |
| (1,3670) | 1:B:105:ALA:H | 1:B:106:PRO:HD3 | 10 | 0.12 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD21 | 5 | 0.12 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD22 | 5 | 0.12 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD23 | 5 | 0.12 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD21 | 6 | 0.12 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD22 | 6 | 0.12 |
| (1,3665) | 1:B:103:HIS:H | 1:B:109:LEU:HD23 | 6 | 0.12 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD11 | 9 | 0.12 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD12 | 9 | 0.12 |
| (1,3661) | 1:B:102:ASN:HD22 | 1:B:157:LEU:HD13 | 9 | 0.12 |
| (1,3655) | 1:B:102:ASN:HD21 | 1:B:161:GLY:HA3 | 10 | 0.12 |
| (1,3651) | 1:B:102:ASN:HD21 | 1:B:109:LEU:HD21 | 10 | 0.12 |
| (1,3651) | 1:B:102:ASN:HD21 | 1:B:109:LEU:HD22 | 10 | 0.12 |
| (1,3651) | 1:B:102:ASN:HD21 | 1:B:109:LEU:HD23 | 10 | 0.12 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD11 | 3 | 0.12 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD12 | 3 | 0.12 |
| (1,364) | 1:A:109:LEU:HG | 1:A:120:ILE:HD13 | 3 | 0.12 |
| (1,3592) | 1:B:170:PRO:HB2 | 1:B:170:PRO:HG2 | 3 | 0.12 |
| (1,3592) | 1:B:170:PRO:HB2 | 1:B:170:PRO:HG2 | 9 | 0.12 |
| (1,359) | 1:A:109:LEU:HB2 | 1:A:122:GLY:HA2 | 8 | 0.12 |
| (1,3561) | 1:B:168:PRO:HB2 | 1:B:170:PRO:HD2 | 4 | 0.12 |
| (1,3561) | 1:B:168:PRO:HB2 | 1:B:170:PRO:HD3 | 4 | 0.12 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD2 | 4 | 0.12 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD2 | 4 | 0.12 |
| (1,3541) | 1:B:166:GLU:HG2 | 1:B:168:PRO:HD3 | 4 | 0.12 |
| (1,3541) | 1:B:166:GLU:HG3 | 1:B:168:PRO:HD3 | 4 | 0.12 |
| (1,35) | 1:A:94:ARG:HB2 | 1:A:94:ARG:HG3 | 8 | 0.12 |
| (1,3498) | 1:B:161:GLY:HA3 | 1:B:163:LEU:HA | 5 | 0.12 |
| (1,3487) | 1:B:159:PRO:HD2 | 1:B:160:GLU:HB3 | 7 | 0.12 |
| (1,3455) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HG | 4 | 0.12 |
| (1,3455) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HG | 4 | 0.12 |
| (1,3455) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HG | 4 | 0.12 |
| (1,3438) | 1:B:157:LEU:HB3 | 1:B:157:LEU:HG | 10 | 0.12 |
| (1,3436) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HA | 3 | 0.12 |
| (1,3423) | 1:B:156:SER:HB3 | 1:B:164:THR:HG21 | 3 | 0.12 |
| (1,3423) | 1:B:156:SER:HB3 | 1:B:164:THR:HG22 | 3 | 0.12 |
| (1,3423) | 1:B:156:SER:HB3 | 1:B:164:THR:HG23 | 3 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD11 | 1 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD12 | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD13 | 1 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD21 | 1 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD22 | 1 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD23 | 1 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD11 | 8 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD12 | 8 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD13 | 8 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD21 | 8 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD22 | 8 | 0.12 |
| (1,3387) | 1:B:155:SER:HA | 1:B:163:LEU:HD23 | 8 | 0.12 |
| (1,3378) | 1:B:154:SER:HB3 | 1:B:155:SER:HA | 3 | 0.12 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG3 | 6 | 0.12 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG2 | 6 | 0.12 |
| (1,3360) | 1:B:153:VAL:HB | 1:B:154:SER:HA | 6 | 0.12 |
| (1,3288) | 1:B:148:VAL:HG11 | 1:B:153:VAL:HA | 3 | 0.12 |
| (1,3288) | 1:B:148:VAL:HG12 | 1:B:153:VAL:HA | 3 | 0.12 |
| (1,3288) | 1:B:148:VAL:HG13 | 1:B:153:VAL:HA | 3 | 0.12 |
| (1,3288) | 1:B:148:VAL:HG11 | 1:B:153:VAL:HA | 8 | 0.12 |
| (1,3288) | 1:B:148:VAL:HG12 | 1:B:153:VAL:HA | 8 | 0.12 |
| (1,3288) | 1:B:148:VAL:HG13 | 1:B:153:VAL:HA | 8 | 0.12 |
| (1,3249) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA3 | 10 | 0.12 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG11 | 5 | 0.12 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG12 | 5 | 0.12 |
| (1,3240) | 1:B:145:PRO:HG3 | 1:B:148:VAL:HG13 | 5 | 0.12 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG11 | 5 | 0.12 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG12 | 5 | 0.12 |
| (1,3240) | 1:B:145:PRO:HG2 | 1:B:148:VAL:HG13 | 5 | 0.12 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 7 | 0.12 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 7 | 0.12 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 7 | 0.12 |
| (1,3186) | 1:B:144:LEU:HA | 1:B:145:PRO:HG3 | 3 | 0.12 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD11 | 8 | 0.12 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD12 | 8 | 0.12 |
| (1,3177) | 1:B:143:THR:HB | 1:B:144:LEU:HD13 | 8 | 0.12 |
| (1,3115) | 1:B:139:THR:HG21 | 1:B:140:ARG:HG2 | 2 | 0.12 |
| (1,3115) | 1:B:139:THR:HG22 | 1:B:140:ARG:HG2 | 2 | 0.12 |
| (1,3115) | 1:B:139:THR:HG23 | 1:B:140:ARG:HG2 | 2 | 0.12 |
| (1,3115) | 1:B:139:THR:HG21 | 1:B:140:ARG:HG3 | 2 | 0.12 |
| (1,3115) | 1:B:139:THR:HG22 | 1:B:140:ARG:HG3 | 2 | 0.12 |
| (1,3115) | 1:B:139:THR:HG23 | 1:B:140:ARG:HG3 | 2 | 0.12 |
| (1,3056) | 1:B:130:GLU:HG2 | 1:B:131:HIS:HD2 | 3 | 0.12 |
| (1,3037) | 1:B:128:GLN:HB3 | 1:B:133:TYR:HD1 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3037) | 1:B:128:GLN:HB3 | 1:B:133:TYR:HD2 | 4 | 0.12 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE1 | 4 | 0.12 |
| (1,3035) | 1:B:128:GLN:HB2 | 1:B:133:TYR:HE2 | 4 | 0.12 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE1 | 4 | 0.12 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE2 | 4 | 0.12 |
| (1,2997) | 1:B:126:GLU:HG2 | 1:B:127:ARG:HG2 | 6 | 0.12 |
| (1,2952) | 1:B:121:THR:HG21 | 1:B:137:CYS:HB3 | 3 | 0.12 |
| (1,2952) | 1:B:121:THR:HG22 | 1:B:137:CYS:HB3 | 3 | 0.12 |
| (1,2952) | 1:B:121:THR:HG23 | 1:B:137:CYS:HB3 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD11 | 1:B:163:LEU:HD11 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD11 | 1:B:163:LEU:HD12 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD11 | 1:B:163:LEU:HD13 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD12 | 1:B:163:LEU:HD11 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD12 | 1:B:163:LEU:HD12 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD12 | 1:B:163:LEU:HD13 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD13 | 1:B:163:LEU:HD11 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD13 | 1:B:163:LEU:HD12 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD13 | 1:B:163:LEU:HD13 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD11 | 1:B:163:LEU:HD21 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD11 | 1:B:163:LEU:HD22 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD11 | 1:B:163:LEU:HD23 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD12 | 1:B:163:LEU:HD21 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD12 | 1:B:163:LEU:HD22 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD12 | 1:B:163:LEU:HD23 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD13 | 1:B:163:LEU:HD21 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD13 | 1:B:163:LEU:HD22 | 3 | 0.12 |
| (1,2941) | 1:B:120:ILE:HD13 | 1:B:163:LEU:HD23 | 3 | 0.12 |
| (1,2935) | 1:B:120:ILE:HD11 | 1:B:140:ARG:HD2 | 8 | 0.12 |
| (1,2935) | 1:B:120:ILE:HD12 | 1:B:140:ARG:HD2 | 8 | 0.12 |
| (1,2935) | 1:B:120:ILE:HD13 | 1:B:140:ARG:HD2 | 8 | 0.12 |
| (1,29) | 1:A:94:ARG:HA | 1:A:168:PRO:HA | 10 | 0.12 |
| (1,2892) | 1:B:119:GLU:HA | 1:B:141:LYS:HE2 | 2 | 0.12 |
| (1,2892) | 1:B:119:GLU:HA | 1:B:141:LYS:HE2 | 8 | 0.12 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 7 | 0.12 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 7 | 0.12 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 7 | 0.12 |
| (1,2886) | 1:B:119:GLU:HA | 1:B:120:ILE:HG13 | 7 | 0.12 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD21 | 8 | 0.12 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD22 | 8 | 0.12 |
| (1,2869) | 1:B:118:VAL:HG11 | 1:B:144:LEU:HD23 | 8 | 0.12 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD21 | 8 | 0.12 |
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD22 | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2869) | 1:B:118:VAL:HG12 | 1:B:144:LEU:HD23 | 8 | 0.12 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD21 | 8 | 0.12 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD22 | 8 | 0.12 |
| (1,2869) | 1:B:118:VAL:HG13 | 1:B:144:LEU:HD23 | 8 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG11 | 1:B:142:TYR:HD1 | 2 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG11 | 1:B:142:TYR:HD2 | 2 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG12 | 1:B:142:TYR:HD1 | 2 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG12 | 1:B:142:TYR:HD2 | 2 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG13 | 1:B:142:TYR:HD1 | 2 | 0.12 |
| (1,2866) | 1:B:118:VAL:HG13 | 1:B:142:TYR:HD2 | 2 | 0.12 |
| (1,2844) | 1:B:118:VAL:HA | 1:B:118:VAL:HG11 | 2 | 0.12 |
| (1,2844) | 1:B:118:VAL:HA | 1:B:118:VAL:HG12 | 2 | 0.12 |
| (1,2844) | 1:B:118:VAL:HA | 1:B:118:VAL:HG13 | 2 | 0.12 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 3 | 0.12 |
| (1,283) | 1:A:105:ALA:HA | 1:A:106:PRO:HB3 | 10 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG21 | 1 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG22 | 1 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG23 | 1 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG21 | 5 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG22 | 5 | 0.12 |
| (1,2827) | 1:B:117:VAL:HA | 1:B:143:THR:HG23 | 5 | 0.12 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG11 | 5 | 0.12 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG12 | 5 | 0.12 |
| (1,2810) | 1:B:116:GLY:HA2 | 1:B:148:VAL:HG13 | 5 | 0.12 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG21 | 7 | 0.12 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG22 | 7 | 0.12 |
| (1,2802) | 1:B:116:GLY:HA2 | 1:B:118:VAL:HG23 | 7 | 0.12 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 4 | 0.12 |
| (1,280) | 1:A:102:ASN:HB3 | 1:A:161:GLY:HA3 | 6 | 0.12 |
| (1,2798) | 1:B:115:ASP:HB3 | 1:B:150:PRO:HG2 | 7 | 0.12 |
| (1,2798) | 1:B:115:ASP:HB3 | 1:B:150:PRO:HG2 | 10 | 0.12 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG11 | 7 | 0.12 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG12 | 7 | 0.12 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG13 | 7 | 0.12 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG21 | 7 | 0.12 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG22 | 7 | 0.12 |
| (1,2766) | 1:B:113:THR:HA | 1:B:153:VAL:HG23 | 7 | 0.12 |
| (1,2752) | 1:B:112:LYS:HD2 | 1:B:114:LYS:HA | 1 | 0.12 |
| (1,2752) | 1:B:112:LYS:HD3 | 1:B:114:LYS:HA | 1 | 0.12 |
| (1,2751) | 1:B:112:LYS:HD2 | 1:B:113:THR:HA | 4 | 0.12 |
| (1,2751) | 1:B:112:LYS:HD3 | 1:B:113:THR:HA | 4 | 0.12 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD11 | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD12 | 1 | 0.12 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD13 | 1 | 0.12 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD21 | 1 | 0.12 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD22 | 1 | 0.12 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD23 | 1 | 0.12 |
| (1,2699) | 1:B:111:VAL:HA | 1:B:120:ILE:HG12 | 4 | 0.12 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG2 | 10 | 0.12 |
| (1,2676) | 1:B:110:THR:HB | 1:B:112:LYS:HG3 | 10 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 1 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 7 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 7 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 7 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 7 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 7 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 7 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 7 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 7 | 0.12 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 7 | 0.12 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD21 | 10 | 0.12 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD22 | 10 | 0.12 |
| (1,2642) | 1:B:109:LEU:HB3 | 1:B:109:LEU:HD23 | 10 | 0.12 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG21 | 4 | 0.12 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG22 | 4 | 0.12 |
| (1,262) | 1:A:100:ASP:HA | 1:A:162:THR:HG23 | 4 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB1 | 1:B:109:LEU:HD21 | 10 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB1 | 1:B:109:LEU:HD22 | 10 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB1 | 1:B:109:LEU:HD23 | 10 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB2 | 1:B:109:LEU:HD21 | 10 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB2 | 1:B:109:LEU:HD22 | 10 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB2 | 1:B:109:LEU:HD23 | 10 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB3 | 1:B:109:LEU:HD21 | 10 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB3 | 1:B:109:LEU:HD22 | 10 | 0.12 |
| (1,2582) | 1:B:105:ALA:HB3 | 1:B:109:LEU:HD23 | 10 | 0.12 |
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD11 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD12 | 6 | 0.12 |
| (1,2569) | 1:B:105:ALA:HA | 1:B:109:LEU:HD13 | 6 | 0.12 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD11 | 10 | 0.12 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD12 | 10 | 0.12 |
| (1,2557) | 1:B:102:ASN:HB2 | 1:B:157:LEU:HD13 | 10 | 0.12 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG21 | 2 | 0.12 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG22 | 2 | 0.12 |
| (1,2543) | 1:B:100:ASP:HA | 1:B:162:THR:HG23 | 2 | 0.12 |
| (1,253) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HD1 | 10 | 0.12 |
| (1,253) | 1:A:99:LEU:HD21 | 1:A:142:TYR:HD2 | 10 | 0.12 |
| (1,253) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HD1 | 10 | 0.12 |
| (1,253) | 1:A:99:LEU:HD22 | 1:A:142:TYR:HD2 | 10 | 0.12 |
| (1,253) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HD1 | 10 | 0.12 |
| (1,253) | 1:A:99:LEU:HD23 | 1:A:142:TYR:HD2 | 10 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG21 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG22 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG23 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG21 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG22 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG23 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG21 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG22 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG23 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG11 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG12 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD21 | 1:B:101:VAL:HG13 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG11 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG12 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD22 | 1:B:101:VAL:HG13 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG11 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG12 | 6 | 0.12 |
| (1,2519) | 1:B:99:LEU:HD23 | 1:B:101:VAL:HG13 | 6 | 0.12 |
| (1,2493) | 1:B:99:LEU:HB2 | 1:B:109:LEU:HD21 | 6 | 0.12 |
| (1,2493) | 1:B:99:LEU:HB2 | 1:B:109:LEU:HD22 | 6 | 0.12 |
| (1,2493) | 1:B:99:LEU:HB2 | 1:B:109:LEU:HD23 | 6 | 0.12 |
| (1,2442) | 1:B:97:VAL:HG21 | 1:B:166:GLU:HA | 7 | 0.12 |
| (1,2442) | 1:B:97:VAL:HG22 | 1:B:166:GLU:HA | 7 | 0.12 |
| (1,2442) | 1:B:97:VAL:HG23 | 1:B:166:GLU:HA | 7 | 0.12 |
| (1,2381) | 1:B:96:ARG:HB3 | 1:B:164:THR:HG21 | 3 | 0.12 |
| (1,2381) | 1:B:96:ARG:HB3 | 1:B:164:THR:HG22 | 3 | 0.12 |
| (1,2381) | 1:B:96:ARG:HB3 | 1:B:164:THR:HG23 | 3 | 0.12 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG21 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG22 | 6 | 0.12 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG23 | 6 | 0.12 |
| (1,2360) | 1:B:96:ARG:HA | 1:B:96:ARG:HG3 | 8 | 0.12 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG11 | 5 | 0.12 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG12 | 5 | 0.12 |
| (1,2343) | 1:B:95:TRP:HB2 | 1:B:148:VAL:HG13 | 5 | 0.12 |
| (1,2330) | 1:B:94:ARG:HD3 | 1:B:168:PRO:HA | 7 | 0.12 |
| (1,2323) | 1:B:94:ARG:HB3 | 1:B:168:PRO:HA | 2 | 0.12 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD3 | 4 | 0.12 |
| (1,2320) | 1:B:94:ARG:HB3 | 1:B:94:ARG:HD2 | 4 | 0.12 |
| (1,23) | 1:A:94:ARG:HA | 1:A:94:ARG:HB3 | 9 | 0.12 |
| (1,2291) | 1:B:91:THR:HA | 1:B:91:THR:HB | 2 | 0.12 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 4 | 0.12 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 4 | 0.12 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 4 | 0.12 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 4 | 0.12 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG21 | 2 | 0.12 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG22 | 2 | 0.12 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG23 | 2 | 0.12 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG21 | 6 | 0.12 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG22 | 6 | 0.12 |
| (1,2230) | 1:B:135:SER:HB2 | 1:A:139:THR:HG23 | 6 | 0.12 |
| (1,2225) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 9 | 0.12 |
| (1,2225) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 9 | 0.12 |
| (1,2225) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 9 | 0.12 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 2 | 0.12 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 2 | 0.12 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 2 | 0.12 |
| (1,2159) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB2 | 2 | 0.12 |
| (1,2157) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 1 | 0.12 |
| (1,2155) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD1 | 1 | 0.12 |
| (1,2155) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD2 | 1 | 0.12 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 4 | 0.12 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 4 | 0.12 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 4 | 0.12 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 4 | 0.12 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG21 | 2 | 0.12 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG22 | 2 | 0.12 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG23 | 2 | 0.12 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG21 | 6 | 0.12 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG22 | 6 | 0.12 |
| (1,2098) | 1:B:135:SER:HB2 | 1:A:139:THR:HG23 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2093) | 1:A:134:ILE:HD11 | 1:B:140:ARG:HD2 | 9 | 0.12 |
| (1,2093) | 1:A:134:ILE:HD12 | 1:B:140:ARG:HD2 | 9 | 0.12 |
| (1,2093) | 1:A:134:ILE:HD13 | 1:B:140:ARG:HD2 | 9 | 0.12 |
| (1,2027) | 1:B:132:GLY:HA2 | 1:A:142:TYR:HB2 | 2 | 0.12 |
| (1,2025) | 1:B:132:GLY:HA2 | 1:A:140:ARG:HA | 1 | 0.12 |
| (1,2023) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD1 | 1 | 0.12 |
| (1,2023) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD2 | 1 | 0.12 |
| (1,2010) | 1:A:171:LYS:H | 1:A:172:LEU:HA | 5 | 0.12 |
| (1,2000) | 1:A:169:MET:H | 1:A:169:MET:HG3 | 3 | 0.12 |
| (1,1964) | 1:A:166:GLU:H | 1:A:155:SER:HB2 | 2 | 0.12 |
| (1,1964) | 1:A:166:GLU:H | 1:A:155:SER:HB3 | 2 | 0.12 |
| (1,1950) | 1:A:165:VAL:H | 1:A:96:ARG:HB2 | 7 | 0.12 |
| (1,1950) | 1:A:165:VAL:H | 1:A:96:ARG:HB3 | 7 | 0.12 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG21 | 10 | 0.12 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG22 | 10 | 0.12 |
| (1,1914) | 1:A:161:GLY:H | 1:A:162:THR:HG23 | 10 | 0.12 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 1 | 0.12 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 5 | 0.12 |
| (1,1911) | 1:A:161:GLY:H | 1:A:161:GLY:HA2 | 6 | 0.12 |
| (1,1900) | 1:A:160:GLU:H | 1:A:162:THR:HB | 4 | 0.12 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG21 | 5 | 0.12 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG22 | 5 | 0.12 |
| (1,1887) | 1:A:158:SER:H | 1:A:162:THR:HG23 | 5 | 0.12 |
| (1,1870) | 1:A:157:LEU:H | 1:A:157:LEU:HB3 | 10 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG11 | 2 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG12 | 2 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG13 | 2 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG21 | 2 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG22 | 2 | 0.12 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG23 | 2 | 0.12 |
| (1,1849) | 1:A:155:SER:H | 1:A:156:SER:HA | 4 | 0.12 |
| (1,1844) | 1:A:154:SER:H | 1:A:168:PRO:HD2 | 10 | 0.12 |
| (1,1804) | 1:A:152:GLN:HE21 | 1:A:169:MET:HA | 6 | 0.12 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB1 | 6 | 0.12 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB2 | 6 | 0.12 |
| (1,1801) | 1:A:152:GLN:HE21 | 1:A:167:ALA:HB3 | 6 | 0.12 |
| (1,1766) | 1:A:149:ASP:H | 1:A:169:MET:HG3 | 9 | 0.12 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD2 | 6 | 0.12 |
| (1,1757) | 1:A:148:VAL:H | 1:A:170:PRO:HD3 | 6 | 0.12 |
| (1,1745) | 1:A:148:VAL:H | 1:A:146:PRO:HD2 | 9 | 0.12 |
| (1,1745) | 1:A:148:VAL:H | 1:A:146:PRO:HD3 | 9 | 0.12 |
| (1,1743) | 1:A:148:VAL:H | 1:A:146:PRO:HB3 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 7 | 0.12 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 7 | 0.12 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 7 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 3 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 3 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 3 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 3 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 3 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 3 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD11 | 4 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD12 | 4 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD13 | 4 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD21 | 4 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD22 | 4 | 0.12 |
| (1,1690) | 1:A:140:ARG:H | 1:A:99:LEU:HD23 | 4 | 0.12 |
| (1,1656) | 1:A:134:ILE:H | 1:A:127:ARG:HG3 | 7 | 0.12 |
| (1,1655) | 1:A:134:ILE:H | 1:A:127:ARG:HG2 | 9 | 0.12 |
| (1,1647) | 1:A:132:GLY:H | 1:A:131:HIS:HB3 | 8 | 0.12 |
| (1,1642) | 1:A:132:GLY:H | 1:A:129:ASP:HB2 | 1 | 0.12 |
| (1,1627) | 1:A:129:ASP:H | 1:A:132:GLY:H | 2 | 0.12 |
| (1,1627) | 1:A:129:ASP:H | 1:A:132:GLY:H | 8 | 0.12 |
| (1,1624) | 1:A:129:ASP:H | 1:A:131:HIS:HA | 5 | 0.12 |
| (1,161) | 1:A:97:VAL:HG21 | 1:A:166:GLU:HA | 10 | 0.12 |
| (1,161) | 1:A:97:VAL:HG22 | 1:A:166:GLU:HA | 10 | 0.12 |
| (1,161) | 1:A:97:VAL:HG23 | 1:A:166:GLU:HA | 10 | 0.12 |
| (1,1598) | 1:A:128:GLN:H | 1:A:127:ARG:HG2 | 9 | 0.12 |
| (1,1588) | 1:A:126:GLU:H | 1:A:125:GLU:HG3 | 3 | 0.12 |
| (1,1569) | 1:A:123:LYS:H | 1:A:109:LEU:HD21 | 2 | 0.12 |
| (1,1569) | 1:A:123:LYS:H | 1:A:109:LEU:HD22 | 2 | 0.12 |
| (1,1569) | 1:A:123:LYS:H | 1:A:109:LEU:HD23 | 2 | 0.12 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 6 | 0.12 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG21 | 1 | 0.12 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG22 | 1 | 0.12 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG23 | 1 | 0.12 |
| (1,1554) | 1:A:121:THR:H | 1:A:120:ILE:HG21 | 2 | 0.12 |
| (1,1554) | 1:A:121:THR:H | 1:A:120:ILE:HG22 | 2 | 0.12 |
| (1,1554) | 1:A:121:THR:H | 1:A:120:ILE:HG23 | 2 | 0.12 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG21 | 8 | 0.12 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG22 | 8 | 0.12 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG23 | 8 | 0.12 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG11 | 8 | 0.12 |
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG12 | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1550) | 1:A:121:THR:H | 1:A:111:VAL:HG13 | 8 | 0.12 |
| (1,1545) | 1:A:120:ILE:H | 1:A:140:ARG:HG3 | 1 | 0.12 |
| (1,1543) | 1:A:120:ILE:H | 1:A:140:ARG:HB2 | 10 | 0.12 |
| (1,1543) | 1:A:120:ILE:H | 1:A:140:ARG:HB3 | 10 | 0.12 |
| (1,1517) | 1:A:118:VAL:H | 1:A:142:TYR:HB2 | 3 | 0.12 |
| (1,1445) | 1:A:111:VAL:H | 1:A:110:THR:HB | 9 | 0.12 |
| (1,1428) | 1:A:109:LEU:H | 1:A:109:LEU:HB3 | 4 | 0.12 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD1 | 7 | 0.12 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD2 | 7 | 0.12 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD1 | 7 | 0.12 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD2 | 7 | 0.12 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD1 | 7 | 0.12 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD2 | 7 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD21 | 3 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD22 | 3 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD23 | 3 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD21 | 3 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD22 | 3 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD23 | 3 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD21 | 6 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD22 | 6 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:157:LEU:HD23 | 6 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD21 | 6 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD22 | 6 | 0.12 |
| (1,1409) | 1:A:107:ASP:H | 1:A:109:LEU:HD23 | 6 | 0.12 |
| (1,1382) | 1:A:102:ASN:HD22 | 1:A:161:GLY:HA2 | 10 | 0.12 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB2 | 8 | 0.12 |
| (1,1360) | 1:A:101:VAL:H | 1:A:100:ASP:HB3 | 8 | 0.12 |
| (1,1345) | 1:A:97:VAL:H | 1:A:165:VAL:H | 1 | 0.12 |
| (1,1327) | 1:A:94:ARG:H | 1:A:169:MET:HG2 | 10 | 0.12 |
| (1,1311) | 1:A:170:PRO:HB2 | 1:A:170:PRO:HG2 | 7 | 0.12 |
| (1,1287) | 1:A:169:MET:HA | 1:A:169:MET:HB3 | 10 | 0.12 |
| (1,1277) | 1:A:168:PRO:HA | 1:A:169:MET:HG3 | 8 | 0.12 |
| (1,1258) | 1:A:166:GLU:HG2 | 1:A:167:ALA:HA | 4 | 0.12 |
| (1,1258) | 1:A:166:GLU:HG3 | 1:A:167:ALA:HA | 4 | 0.12 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG2 | 1 | 0.12 |
| (1,1240) | 1:A:164:THR:HB | 1:A:166:GLU:HG3 | 1 | 0.12 |
| (1,1196) | 1:A:158:SER:HB2 | 1:A:159:PRO:HD2 | 4 | 0.12 |
| (1,1196) | 1:A:158:SER:HB3 | 1:A:159:PRO:HD2 | 4 | 0.12 |
| (1,1193) | 1:A:158:SER:HB3 | 1:A:160:GLU:HB3 | 7 | 0.12 |
| (1,1173) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB3 | 2 | 0.12 |
| (1,1173) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB3 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1173) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB3 | 2 | 0.12 |
| (1,1172) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB2 | 4 | 0.12 |
| (1,1172) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB2 | 4 | 0.12 |
| (1,1172) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB2 | 4 | 0.12 |
| (1,117) | 1:A:96:ARG:HD2 | 1:A:166:GLU:HG2 | 2 | 0.12 |
| (1,117) | 1:A:96:ARG:HD3 | 1:A:166:GLU:HG3 | 2 | 0.12 |
| (1,117) | 1:A:96:ARG:HD3 | 1:A:166:GLU:HG2 | 2 | 0.12 |
| (1,117) | 1:A:96:ARG:HD2 | 1:A:166:GLU:HG3 | 2 | 0.12 |
| (1,1157) | 1:A:157:LEU:HB3 | 1:A:157:LEU:HG | 4 | 0.12 |
| (1,1149) | 1:A:157:LEU:HA | 1:A:163:LEU:HB3 | 9 | 0.12 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD11 | 3 | 0.12 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD12 | 3 | 0.12 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD13 | 3 | 0.12 |
| (1,1139) | 1:A:156:SER:HB3 | 1:A:157:LEU:HB3 | 3 | 0.12 |
| (1,1079) | 1:A:153:VAL:HB | 1:A:154:SER:HA | 5 | 0.12 |
| (1,1079) | 1:A:153:VAL:HB | 1:A:154:SER:HA | 8 | 0.12 |
| (1,1036) | 1:A:150:PRO:HA | 1:A:151:THR:HG21 | 4 | 0.12 |
| (1,1036) | 1:A:150:PRO:HA | 1:A:151:THR:HG22 | 4 | 0.12 |
| (1,1036) | 1:A:150:PRO:HA | 1:A:151:THR:HG23 | 4 | 0.12 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG21 | 3 | 0.11 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG22 | 3 | 0.11 |
| (1,938) | 1:A:144:LEU:HD21 | 1:A:148:VAL:HG23 | 3 | 0.11 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG21 | 3 | 0.11 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG22 | 3 | 0.11 |
| (1,938) | 1:A:144:LEU:HD22 | 1:A:148:VAL:HG23 | 3 | 0.11 |
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG21 | 3 | 0.11 |
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG22 | 3 | 0.11 |
| (1,938) | 1:A:144:LEU:HD23 | 1:A:148:VAL:HG23 | 3 | 0.11 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG21 | 7 | 0.11 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG22 | 7 | 0.11 |
| (1,913) | 1:A:144:LEU:HB2 | 1:A:148:VAL:HG23 | 7 | 0.11 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG11 | 1 | 0.11 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG12 | 1 | 0.11 |
| (1,882) | 1:A:142:TYR:HD1 | 1:A:165:VAL:HG13 | 1 | 0.11 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG11 | 1 | 0.11 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG12 | 1 | 0.11 |
| (1,882) | 1:A:142:TYR:HD2 | 1:A:165:VAL:HG13 | 1 | 0.11 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 1 | 0.11 |
| (1,842) | 1:A:141:LYS:HA | 1:A:141:LYS:HB2 | 6 | 0.11 |
| (1,779) | 1:A:131:HIS:HA | 1:A:131:HIS:HE1 | 7 | 0.11 |
| (1,759) | 1:A:128:GLN:HG2 | 1:A:133:TYR:HA | 1 | 0.11 |
| (1,759) | 1:A:128:GLN:HG2 | 1:A:133:TYR:HA | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,742) | 1:A:127:ARG:HB2 | 1:A:127:ARG:HD2 | 1 | 0.11 |
| (1,737) | 1:A:127:ARG:HA | 1:A:127:ARG:HD3 | 10 | 0.11 |
| (1,734) | 1:A:127:ARG:HA | 1:A:127:ARG:HB3 | 4 | 0.11 |
| (1,734) | 1:A:127:ARG:HA | 1:A:127:ARG:HB3 | 6 | 0.11 |
| (1,734) | 1:A:127:ARG:HA | 1:A:127:ARG:HB3 | 8 | 0.11 |
| (1,734) | 1:A:127:ARG:HA | 1:A:127:ARG:HB3 | 10 | 0.11 |
| (1,729) | 1:A:126:GLU:HG3 | 1:A:133:TYR:HB3 | 10 | 0.11 |
| (1,719) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HD1 | 2 | 0.11 |
| (1,719) | 1:A:126:GLU:HG2 | 1:A:133:TYR:HD2 | 2 | 0.11 |
| (1,714) | 1:A:126:GLU:HB3 | 1:A:135:SER:HB2 | 2 | 0.11 |
| (1,714) | 1:A:126:GLU:HB2 | 1:A:135:SER:HB2 | 2 | 0.11 |
| (1,708) | 1:A:126:GLU:HA | 1:A:134:ILE:HG21 | 6 | 0.11 |
| (1,708) | 1:A:126:GLU:HA | 1:A:134:ILE:HG22 | 6 | 0.11 |
| (1,708) | 1:A:126:GLU:HA | 1:A:134:ILE:HG23 | 6 | 0.11 |
| (1,704) | 1:A:125:GLU:HA | 1:A:135:SER:HB3 | 2 | 0.11 |
| (1,692) | 1:A:123:LYS:HG3 | 1:A:137:CYS:HB2 | 10 | 0.11 |
| (1,671) | 1:A:121:THR:HG21 | 1:A:137:CYS:HB3 | 2 | 0.11 |
| (1,671) | 1:A:121:THR:HG22 | 1:A:137:CYS:HB3 | 2 | 0.11 |
| (1,671) | 1:A:121:THR:HG23 | 1:A:137:CYS:HB3 | 2 | 0.11 |
| (1,664) | 1:A:121:THR:HA | 1:A:139:THR:HA | 10 | 0.11 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD1 | 6 | 0.11 |
| (1,650) | 1:A:120:ILE:HG21 | 1:A:142:TYR:HD2 | 6 | 0.11 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD1 | 6 | 0.11 |
| (1,650) | 1:A:120:ILE:HG22 | 1:A:142:TYR:HD2 | 6 | 0.11 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD1 | 6 | 0.11 |
| (1,650) | 1:A:120:ILE:HG23 | 1:A:142:TYR:HD2 | 6 | 0.11 |
| (1,649) | 1:A:120:ILE:HG21 | 1:A:140:ARG:HA | 6 | 0.11 |
| (1,649) | 1:A:120:ILE:HG22 | 1:A:140:ARG:HA | 6 | 0.11 |
| (1,649) | 1:A:120:ILE:HG23 | 1:A:140:ARG:HA | 6 | 0.11 |
| (1,648) | 1:A:120:ILE:HG21 | 1:A:139:THR:HA | 8 | 0.11 |
| (1,648) | 1:A:120:ILE:HG22 | 1:A:139:THR:HA | 8 | 0.11 |
| (1,648) | 1:A:120:ILE:HG23 | 1:A:139:THR:HA | 8 | 0.11 |
| (1,647) | 1:A:120:ILE:HG21 | 1:A:122:GLY:HA3 | 8 | 0.11 |
| (1,647) | 1:A:120:ILE:HG22 | 1:A:122:GLY:HA3 | 8 | 0.11 |
| (1,647) | 1:A:120:ILE:HG23 | 1:A:122:GLY:HA3 | 8 | 0.11 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 6 | 0.11 |
| (1,639) | 1:A:120:ILE:HG12 | 1:A:121:THR:HA | 7 | 0.11 |
| (1,636) | 1:A:120:ILE:HB | 1:A:140:ARG:HD3 | 6 | 0.11 |
| (1,604) | 1:A:119:GLU:HA | 1:A:120:ILE:HG12 | 9 | 0.11 |
| (1,60) | 1:A:95:TRP:HB2 | 1:A:95:TRP:HE3 | 8 | 0.11 |
| (1,571) | 1:A:118:VAL:HB | 1:A:142:TYR:HD1 | 8 | 0.11 |
| (1,571) | 1:A:118:VAL:HB | 1:A:142:TYR:HD2 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD21 | 10 | 0.11 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD22 | 10 | 0.11 |
| (1,566) | 1:A:118:VAL:HA | 1:A:144:LEU:HD23 | 10 | 0.11 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 1 | 0.11 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 1 | 0.11 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 1 | 0.11 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG11 | 6 | 0.11 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG12 | 6 | 0.11 |
| (1,551) | 1:A:117:VAL:HA | 1:A:148:VAL:HG13 | 6 | 0.11 |
| (1,502) | 1:A:113:THR:HG21 | 1:A:150:PRO:HB3 | 5 | 0.11 |
| (1,502) | 1:A:113:THR:HG22 | 1:A:150:PRO:HB3 | 5 | 0.11 |
| (1,502) | 1:A:113:THR:HG23 | 1:A:150:PRO:HB3 | 5 | 0.11 |
| (1,502) | 1:A:113:THR:HG21 | 1:A:150:PRO:HB3 | 10 | 0.11 |
| (1,502) | 1:A:113:THR:HG22 | 1:A:150:PRO:HB3 | 10 | 0.11 |
| (1,502) | 1:A:113:THR:HG23 | 1:A:150:PRO:HB3 | 10 | 0.11 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG11 | 4 | 0.11 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG12 | 4 | 0.11 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG13 | 4 | 0.11 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG21 | 4 | 0.11 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG22 | 4 | 0.11 |
| (1,485) | 1:A:113:THR:HA | 1:A:153:VAL:HG23 | 4 | 0.11 |
| (1,484) | 1:A:113:THR:HA | 1:A:118:VAL:HG11 | 4 | 0.11 |
| (1,484) | 1:A:113:THR:HA | 1:A:118:VAL:HG12 | 4 | 0.11 |
| (1,484) | 1:A:113:THR:HA | 1:A:118:VAL:HG13 | 4 | 0.11 |
| (1,475) | 1:A:112:LYS:HE2 | 1:A:119:GLU:HG2 | 3 | 0.11 |
| (1,475) | 1:A:112:LYS:HE3 | 1:A:119:GLU:HG2 | 3 | 0.11 |
| (1,432) | 1:A:111:VAL:HG11 | 1:A:118:VAL:HG21 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG11 | 1:A:118:VAL:HG22 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG11 | 1:A:118:VAL:HG23 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG12 | 1:A:118:VAL:HG21 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG12 | 1:A:118:VAL:HG22 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG12 | 1:A:118:VAL:HG23 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG13 | 1:A:118:VAL:HG21 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG13 | 1:A:118:VAL:HG22 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG13 | 1:A:118:VAL:HG23 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG21 | 1:A:118:VAL:HG21 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG21 | 1:A:118:VAL:HG22 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG21 | 1:A:118:VAL:HG23 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG22 | 1:A:118:VAL:HG21 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG22 | 1:A:118:VAL:HG22 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG22 | 1:A:118:VAL:HG23 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG23 | 1:A:118:VAL:HG21 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,432) | 1:A:111:VAL:HG23 | 1:A:118:VAL:HG22 | 7 | 0.11 |
| (1,432) | 1:A:111:VAL:HG23 | 1:A:118:VAL:HG23 | 7 | 0.11 |
| (1,4263) | 1:B:167:ALA:H | 1:B:166:GLU:HB3 | 1 | 0.11 |
| (1,4197) | 1:B:162:THR:H | 1:B:102:ASN:HB3 | 1 | 0.11 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 1 | 0.11 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 3 | 0.11 |
| (1,4192) | 1:B:161:GLY:H | 1:B:161:GLY:HA2 | 9 | 0.11 |
| (1,4182) | 1:B:161:GLY:H | 1:B:102:ASN:HB2 | 8 | 0.11 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD11 | 6 | 0.11 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD12 | 6 | 0.11 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD13 | 6 | 0.11 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD21 | 6 | 0.11 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD22 | 6 | 0.11 |
| (1,4171) | 1:B:158:SER:H | 1:B:163:LEU:HD23 | 6 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG11 | 2 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG12 | 2 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG13 | 2 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG21 | 2 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG22 | 2 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG23 | 2 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG11 | 3 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG12 | 3 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG13 | 3 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG21 | 3 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG22 | 3 | 0.11 |
| (1,4146) | 1:B:156:SER:H | 1:B:165:VAL:HG23 | 3 | 0.11 |
| (1,413) | 1:A:111:VAL:HA | 1:A:112:LYS:HG2 | 3 | 0.11 |
| (1,413) | 1:A:111:VAL:HA | 1:A:112:LYS:HG3 | 3 | 0.11 |
| (1,4128) | 1:B:155:SER:H | 1:B:154:SER:HB2 | 2 | 0.11 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB1 | 6 | 0.11 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB2 | 6 | 0.11 |
| (1,4124) | 1:B:154:SER:H | 1:B:167:ALA:HB3 | 6 | 0.11 |
| (1,4044) | 1:B:149:ASP:H | 1:B:152:GLN:HB3 | 7 | 0.11 |
| (1,4043) | 1:B:149:ASP:H | 1:B:152:GLN:HB2 | 5 | 0.11 |
| (1,4034) | 1:B:148:VAL:H | 1:B:149:ASP:H | 3 | 0.11 |
| (1,4034) | 1:B:148:VAL:H | 1:B:149:ASP:H | 10 | 0.11 |
| (1,3963) | 1:B:137:CYS:H | 1:B:138:PHE:HE1 | 4 | 0.11 |
| (1,3963) | 1:B:137:CYS:H | 1:B:138:PHE:HE2 | 4 | 0.11 |
| (1,395) | 1:A:110:THR:HB | 1:A:112:LYS:HG2 | 10 | 0.11 |
| (1,395) | 1:A:110:THR:HB | 1:A:112:LYS:HG3 | 10 | 0.11 |
| (1,3936) | 1:B:134:ILE:H | 1:B:127:ARG:HG2 | 7 | 0.11 |
| (1,3936) | 1:B:134:ILE:H | 1:B:127:ARG:HG2 | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG21 | 5 | 0.11 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG22 | 5 | 0.11 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG23 | 5 | 0.11 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG11 | 5 | 0.11 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG12 | 5 | 0.11 |
| (1,393) | 1:A:110:THR:HB | 1:A:111:VAL:HG13 | 5 | 0.11 |
| (1,3928) | 1:B:132:GLY:H | 1:B:131:HIS:HB3 | 3 | 0.11 |
| (1,3919) | 1:B:131:HIS:H | 1:B:132:GLY:HA3 | 2 | 0.11 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB2 | 3 | 0.11 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB3 | 3 | 0.11 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB2 | 9 | 0.11 |
| (1,3917) | 1:B:131:HIS:H | 1:B:130:GLU:HB3 | 9 | 0.11 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD3 | 1 | 0.11 |
| (1,39) | 1:A:94:ARG:HB3 | 1:A:94:ARG:HD2 | 1 | 0.11 |
| (1,3879) | 1:B:128:GLN:H | 1:B:127:ARG:HG2 | 2 | 0.11 |
| (1,3872) | 1:B:126:GLU:H | 1:B:135:SER:HB2 | 10 | 0.11 |
| (1,3872) | 1:B:126:GLU:H | 1:B:135:SER:HB3 | 10 | 0.11 |
| (1,3869) | 1:B:126:GLU:H | 1:B:125:GLU:HG3 | 2 | 0.11 |
| (1,3866) | 1:B:126:GLU:H | 1:B:125:GLU:HA | 5 | 0.11 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD21 | 7 | 0.11 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD22 | 7 | 0.11 |
| (1,3850) | 1:B:123:LYS:H | 1:B:109:LEU:HD23 | 7 | 0.11 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB1 | 2 | 0.11 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB2 | 2 | 0.11 |
| (1,3844) | 1:B:123:LYS:H | 1:B:105:ALA:HB3 | 2 | 0.11 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG21 | 10 | 0.11 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG22 | 10 | 0.11 |
| (1,3837) | 1:B:121:THR:H | 1:B:121:THR:HG23 | 10 | 0.11 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD11 | 4 | 0.11 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD12 | 4 | 0.11 |
| (1,3821) | 1:B:120:ILE:H | 1:B:120:ILE:HD13 | 4 | 0.11 |
| (1,3805) | 1:B:119:GLU:H | 1:B:114:LYS:HB2 | 4 | 0.11 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 5 | 0.11 |
| (1,3790) | 1:B:117:VAL:H | 1:B:144:LEU:H | 9 | 0.11 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB2 | 8 | 0.11 |
| (1,3743) | 1:B:112:LYS:H | 1:B:119:GLU:HB3 | 8 | 0.11 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG21 | 4 | 0.11 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG22 | 4 | 0.11 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG23 | 4 | 0.11 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG11 | 4 | 0.11 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG12 | 4 | 0.11 |
| (1,3737) | 1:B:112:LYS:H | 1:B:111:VAL:HG13 | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3726) | 1:B:111:VAL:H | 1:B:110:THR:HB | 2 | 0.11 |
| (1,3723) | 1:B:110:THR:H | 1:B:122:GLY:H | 5 | 0.11 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD21 | 8 | 0.11 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD22 | 8 | 0.11 |
| (1,371) | 1:A:109:LEU:HD11 | 1:A:157:LEU:HD23 | 8 | 0.11 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD21 | 8 | 0.11 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD22 | 8 | 0.11 |
| (1,371) | 1:A:109:LEU:HD12 | 1:A:157:LEU:HD23 | 8 | 0.11 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD21 | 8 | 0.11 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD22 | 8 | 0.11 |
| (1,371) | 1:A:109:LEU:HD13 | 1:A:157:LEU:HD23 | 8 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 2 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 2 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 2 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 2 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 2 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 2 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 5 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 5 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 5 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 5 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 5 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 5 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD21 | 7 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD22 | 7 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:157:LEU:HD23 | 7 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD21 | 7 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD22 | 7 | 0.11 |
| (1,3690) | 1:B:107:ASP:H | 1:B:109:LEU:HD23 | 7 | 0.11 |
| (1,3670) | 1:B:105:ALA:H | 1:B:106:PRO:HD3 | 9 | 0.11 |
| (1,3643) | 1:B:101:VAL:H | 1:B:120:ILE:HG21 | 9 | 0.11 |
| (1,3643) | 1:B:101:VAL:H | 1:B:120:ILE:HG22 | 9 | 0.11 |
| (1,3643) | 1:B:101:VAL:H | 1:B:120:ILE:HG23 | 9 | 0.11 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG11 | 7 | 0.11 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG12 | 7 | 0.11 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG13 | 7 | 0.11 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG21 | 7 | 0.11 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG22 | 7 | 0.11 |
| (1,3638) | 1:B:99:LEU:H | 1:B:101:VAL:HG23 | 7 | 0.11 |
| (1,3626) | 1:B:97:VAL:H | 1:B:165:VAL:H | 6 | 0.11 |
| (1,3592) | 1:B:170:PRO:HB2 | 1:B:170:PRO:HG2 | 2 | 0.11 |
| (1,3592) | 1:B:170:PRO:HB2 | 1:B:170:PRO:HG2 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3592) | 1:B:170:PRO:HB2 | 1:B:170:PRO:HG2 | 6 | 0.11 |
| (1,3592) | 1:B:170:PRO:HB2 | 1:B:170:PRO:HG2 | 10 | 0.11 |
| (1,3568) | 1:B:169:MET:HA | 1:B:169:MET:HB3 | 6 | 0.11 |
| (1,3563) | 1:B:168:PRO:HB3 | 1:B:169:MET:HA | 2 | 0.11 |
| (1,3481) | 1:B:159:PRO:HA | 1:B:159:PRO:HG3 | 4 | 0.11 |
| (1,3474) | 1:B:158:SER:HB3 | 1:B:160:GLU:HB3 | 5 | 0.11 |
| (1,3455) | 1:B:157:LEU:HD11 | 1:B:163:LEU:HG | 7 | 0.11 |
| (1,3455) | 1:B:157:LEU:HD12 | 1:B:163:LEU:HG | 7 | 0.11 |
| (1,3455) | 1:B:157:LEU:HD13 | 1:B:163:LEU:HG | 7 | 0.11 |
| (1,3436) | 1:B:157:LEU:HB2 | 1:B:163:LEU:HA | 5 | 0.11 |
| (1,3395) | 1:B:155:SER:HB2 | 1:B:163:LEU:HA | 9 | 0.11 |
| (1,3391) | 1:B:155:SER:HA | 1:B:165:VAL:HA | 5 | 0.11 |
| (1,3391) | 1:B:155:SER:HA | 1:B:165:VAL:HA | 10 | 0.11 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG3 | 5 | 0.11 |
| (1,3377) | 1:B:154:SER:HB2 | 1:B:166:GLU:HG2 | 5 | 0.11 |
| (1,3345) | 1:B:152:GLN:HB2 | 1:B:168:PRO:HD3 | 9 | 0.11 |
| (1,332) | 1:A:107:ASP:HA | 1:A:108:GLU:HG3 | 3 | 0.11 |
| (1,3292) | 1:B:148:VAL:HG11 | 1:B:169:MET:HA | 3 | 0.11 |
| (1,3292) | 1:B:148:VAL:HG12 | 1:B:169:MET:HA | 3 | 0.11 |
| (1,3292) | 1:B:148:VAL:HG13 | 1:B:169:MET:HA | 3 | 0.11 |
| (1,3292) | 1:B:148:VAL:HG11 | 1:B:169:MET:HA | 10 | 0.11 |
| (1,3292) | 1:B:148:VAL:HG12 | 1:B:169:MET:HA | 10 | 0.11 |
| (1,3292) | 1:B:148:VAL:HG13 | 1:B:169:MET:HA | 10 | 0.11 |
| (1,3288) | 1:B:148:VAL:HG11 | 1:B:153:VAL:HA | 1 | 0.11 |
| (1,3288) | 1:B:148:VAL:HG12 | 1:B:153:VAL:HA | 1 | 0.11 |
| (1,3288) | 1:B:148:VAL:HG13 | 1:B:153:VAL:HA | 1 | 0.11 |
| (1,3288) | 1:B:148:VAL:HG11 | 1:B:153:VAL:HA | 6 | 0.11 |
| (1,3288) | 1:B:148:VAL:HG12 | 1:B:153:VAL:HA | 6 | 0.11 |
| (1,3288) | 1:B:148:VAL:HG13 | 1:B:153:VAL:HA | 6 | 0.11 |
| (1,3266) | 1:B:148:VAL:HA | 1:B:149:ASP:HB3 | 3 | 0.11 |
| (1,3249) | 1:B:146:PRO:HB3 | 1:B:147:GLY:HA3 | 2 | 0.11 |
| (1,3242) | 1:B:145:PRO:HD2 | 1:B:146:PRO:HB2 | 4 | 0.11 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG21 | 9 | 0.11 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG22 | 9 | 0.11 |
| (1,3194) | 1:B:144:LEU:HB2 | 1:B:148:VAL:HG23 | 9 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD21 | 4 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD22 | 4 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD23 | 4 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD21 | 4 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD22 | 4 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD23 | 4 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD21 | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD22 | 9 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD23 | 9 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD21 | 9 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD22 | 9 | 0.11 |
| (1,3162) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD23 | 9 | 0.11 |
| (1,3161) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD11 | 3 | 0.11 |
| (1,3161) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD12 | 3 | 0.11 |
| (1,3161) | 1:B:142:TYR:HD1 | 1:B:144:LEU:HD13 | 3 | 0.11 |
| (1,3161) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD11 | 3 | 0.11 |
| (1,3161) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD12 | 3 | 0.11 |
| (1,3161) | 1:B:142:TYR:HD2 | 1:B:144:LEU:HD13 | 3 | 0.11 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE1 | 7 | 0.11 |
| (1,3030) | 1:B:128:GLN:HA | 1:B:133:TYR:HE2 | 7 | 0.11 |
| (1,3015) | 1:B:127:ARG:HA | 1:B:127:ARG:HB3 | 2 | 0.11 |
| (1,2975) | 1:B:123:LYS:HD2 | 1:B:137:CYS:HA | 7 | 0.11 |
| (1,2975) | 1:B:123:LYS:HD3 | 1:B:137:CYS:HA | 7 | 0.11 |
| (1,2962) | 1:B:123:LYS:HA | 1:B:123:LYS:HD2 | 4 | 0.11 |
| (1,2962) | 1:B:123:LYS:HA | 1:B:123:LYS:HD3 | 4 | 0.11 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 5 | 0.11 |
| (1,2961) | 1:B:123:LYS:HA | 1:B:123:LYS:HG3 | 7 | 0.11 |
| (1,2933) | 1:B:120:ILE:HD11 | 1:B:140:ARG:HB2 | 9 | 0.11 |
| (1,2933) | 1:B:120:ILE:HD12 | 1:B:140:ARG:HB2 | 9 | 0.11 |
| (1,2933) | 1:B:120:ILE:HD13 | 1:B:140:ARG:HB2 | 9 | 0.11 |
| (1,2920) | 1:B:120:ILE:HG12 | 1:B:121:THR:HA | 6 | 0.11 |
| (1,2914) | 1:B:120:ILE:HB | 1:B:120:ILE:HD11 | 4 | 0.11 |
| (1,2914) | 1:B:120:ILE:HB | 1:B:120:ILE:HD12 | 4 | 0.11 |
| (1,2914) | 1:B:120:ILE:HB | 1:B:120:ILE:HD13 | 4 | 0.11 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD11 | 2 | 0.11 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD12 | 2 | 0.11 |
| (1,289) | 1:A:105:ALA:HA | 1:A:157:LEU:HD13 | 2 | 0.11 |
| (1,2886) | 1:B:119:GLU:HA | 1:B:120:ILE:HG13 | 8 | 0.11 |
| (1,2885) | 1:B:119:GLU:HA | 1:B:120:ILE:HG12 | 2 | 0.11 |
| (1,288) | 1:A:105:ALA:HA | 1:A:109:LEU:HD11 | 10 | 0.11 |
| (1,288) | 1:A:105:ALA:HA | 1:A:109:LEU:HD12 | 10 | 0.11 |
| (1,288) | 1:A:105:ALA:HA | 1:A:109:LEU:HD13 | 10 | 0.11 |
| (1,2864) | 1:B:118:VAL:HG11 | 1:B:142:TYR:HB2 | 6 | 0.11 |
| (1,2864) | 1:B:118:VAL:HG12 | 1:B:142:TYR:HB2 | 6 | 0.11 |
| (1,2864) | 1:B:118:VAL:HG13 | 1:B:142:TYR:HB2 | 6 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG11 | 3 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG12 | 3 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG13 | 3 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG21 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG22 | 3 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG23 | 3 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG11 | 4 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG12 | 4 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG13 | 4 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG21 | 4 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG22 | 4 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG23 | 4 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG11 | 5 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG12 | 5 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG13 | 5 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG21 | 5 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG22 | 5 | 0.11 |
| (1,2848) | 1:B:118:VAL:HA | 1:B:153:VAL:HG23 | 5 | 0.11 |
| (1,2831) | 1:B:117:VAL:HA | 1:B:148:VAL:HB | 5 | 0.11 |
| (1,2783) | 1:B:113:THR:HG21 | 1:B:150:PRO:HB3 | 2 | 0.11 |
| (1,2783) | 1:B:113:THR:HG22 | 1:B:150:PRO:HB3 | 2 | 0.11 |
| (1,2783) | 1:B:113:THR:HG23 | 1:B:150:PRO:HB3 | 2 | 0.11 |
| (1,2783) | 1:B:113:THR:HG21 | 1:B:150:PRO:HB3 | 10 | 0.11 |
| (1,2783) | 1:B:113:THR:HG22 | 1:B:150:PRO:HB3 | 10 | 0.11 |
| (1,2783) | 1:B:113:THR:HG23 | 1:B:150:PRO:HB3 | 10 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 1 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 1 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 1 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 1 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 1 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 1 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG21 | 1:B:155:SER:HB2 | 8 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG22 | 1:B:155:SER:HB2 | 8 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG23 | 1:B:155:SER:HB2 | 8 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG11 | 1:B:155:SER:HB2 | 8 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG12 | 1:B:155:SER:HB2 | 8 | 0.11 |
| (1,2720) | 1:B:111:VAL:HG13 | 1:B:155:SER:HB2 | 8 | 0.11 |
| (1,271) | 1:A:101:VAL:HG21 | 1:A:102:ASN:HA | 8 | 0.11 |
| (1,271) | 1:A:101:VAL:HG22 | 1:A:102:ASN:HA | 8 | 0.11 |
| (1,271) | 1:A:101:VAL:HG23 | 1:A:102:ASN:HA | 8 | 0.11 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD11 | 9 | 0.11 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD12 | 9 | 0.11 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD13 | 9 | 0.11 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD21 | 9 | 0.11 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD22 | 9 | 0.11 |
| (1,2706) | 1:B:111:VAL:HB | 1:B:163:LEU:HD23 | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2694) | 1:B:111:VAL:HA | 1:B:112:LYS:HG2 | 5 | 0.11 |
| (1,2694) | 1:B:111:VAL:HA | 1:B:112:LYS:HG3 | 5 | 0.11 |
| (1,2687) | 1:B:110:THR:HG21 | 1:B:112:LYS:HE2 | 10 | 0.11 |
| (1,2687) | 1:B:110:THR:HG22 | 1:B:112:LYS:HE2 | 10 | 0.11 |
| (1,2687) | 1:B:110:THR:HG23 | 1:B:112:LYS:HE2 | 10 | 0.11 |
| (1,2687) | 1:B:110:THR:HG21 | 1:B:112:LYS:HE3 | 10 | 0.11 |
| (1,2687) | 1:B:110:THR:HG22 | 1:B:112:LYS:HE3 | 10 | 0.11 |
| (1,2687) | 1:B:110:THR:HG23 | 1:B:112:LYS:HE3 | 10 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 1 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 1 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 1 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 1 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 1 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 1 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 7 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 7 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 7 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 7 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 7 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 7 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG21 | 10 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG22 | 10 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG23 | 10 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG11 | 10 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG12 | 10 | 0.11 |
| (1,2674) | 1:B:110:THR:HB | 1:B:111:VAL:HG13 | 10 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD21 | 6 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD22 | 6 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD11 | 1:B:157:LEU:HD23 | 6 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD21 | 6 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD22 | 6 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD12 | 1:B:157:LEU:HD23 | 6 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD21 | 6 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD22 | 6 | 0.11 |
| (1,2652) | 1:B:109:LEU:HD13 | 1:B:157:LEU:HD23 | 6 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD21 | 1 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD22 | 1 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD23 | 1 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD21 | 10 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD22 | 10 | 0.11 |
| (1,2647) | 1:B:109:LEU:HG | 1:B:157:LEU:HD23 | 10 | 0.11 |
| (1,2643) | 1:B:109:LEU:HB3 | 1:B:121:THR:HB | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2626) | 1:B:108:GLU:HG2 | 1:B:123:LYS:HE3 | 6 | 0.11 |
| (1,2626) | 1:B:108:GLU:HG2 | 1:B:123:LYS:HE2 | 6 | 0.11 |
| (1,2617) | 1:B:108:GLU:HA | 1:B:108:GLU:HG2 | 10 | 0.11 |
| (1,261) | 1:A:100:ASP:HA | 1:A:162:THR:HA | 8 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 6 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 6 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 6 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 6 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 6 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 6 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD21 | 8 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD22 | 8 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:109:LEU:HD23 | 8 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD21 | 8 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD22 | 8 | 0.11 |
| (1,2609) | 1:B:106:PRO:HD2 | 1:B:157:LEU:HD23 | 8 | 0.11 |
| (1,2583) | 1:B:105:ALA:HB1 | 1:B:123:LYS:HA | 3 | 0.11 |
| (1,2583) | 1:B:105:ALA:HB2 | 1:B:123:LYS:HA | 3 | 0.11 |
| (1,2583) | 1:B:105:ALA:HB3 | 1:B:123:LYS:HA | 3 | 0.11 |
| (1,258) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HA | 6 | 0.11 |
| (1,258) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HA | 6 | 0.11 |
| (1,258) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HA | 6 | 0.11 |
| (1,258) | 1:A:99:LEU:HD21 | 1:A:120:ILE:HA | 6 | 0.11 |
| (1,258) | 1:A:99:LEU:HD22 | 1:A:120:ILE:HA | 6 | 0.11 |
| (1,258) | 1:A:99:LEU:HD23 | 1:A:120:ILE:HA | 6 | 0.11 |
| (1,258) | 1:A:99:LEU:HD11 | 1:A:120:ILE:HA | 9 | 0.11 |
| (1,258) | 1:A:99:LEU:HD12 | 1:A:120:ILE:HA | 9 | 0.11 |
| (1,258) | 1:A:99:LEU:HD13 | 1:A:120:ILE:HA | 9 | 0.11 |
| (1,258) | 1:A:99:LEU:HD21 | 1:A:120:ILE:HA | 9 | 0.11 |
| (1,258) | 1:A:99:LEU:HD22 | 1:A:120:ILE:HA | 9 | 0.11 |
| (1,258) | 1:A:99:LEU:HD23 | 1:A:120:ILE:HA | 9 | 0.11 |
| (1,2578) | 1:B:105:ALA:HB1 | 1:B:107:ASP:HB3 | 5 | 0.11 |
| (1,2578) | 1:B:105:ALA:HB2 | 1:B:107:ASP:HB3 | 5 | 0.11 |
| (1,2578) | 1:B:105:ALA:HB3 | 1:B:107:ASP:HB3 | 5 | 0.11 |
| (1,2568) | 1:B:105:ALA:HA | 1:B:108:GLU:HB3 | 1 | 0.11 |
| (1,2555) | 1:B:101:VAL:HG11 | 1:B:163:LEU:HG | 1 | 0.11 |
| (1,2555) | 1:B:101:VAL:HG12 | 1:B:163:LEU:HG | 1 | 0.11 |
| (1,2555) | 1:B:101:VAL:HG13 | 1:B:163:LEU:HG | 1 | 0.11 |
| (1,2555) | 1:B:101:VAL:HG21 | 1:B:163:LEU:HG | 1 | 0.11 |
| (1,2555) | 1:B:101:VAL:HG22 | 1:B:163:LEU:HG | 1 | 0.11 |
| (1,2555) | 1:B:101:VAL:HG23 | 1:B:163:LEU:HG | 1 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HA | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2539) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HA | 7 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HA | 7 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD21 | 1:B:120:ILE:HA | 7 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD22 | 1:B:120:ILE:HA | 7 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD23 | 1:B:120:ILE:HA | 7 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD11 | 1:B:120:ILE:HA | 8 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD12 | 1:B:120:ILE:HA | 8 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD13 | 1:B:120:ILE:HA | 8 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD21 | 1:B:120:ILE:HA | 8 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD22 | 1:B:120:ILE:HA | 8 | 0.11 |
| (1,2539) | 1:B:99:LEU:HD23 | 1:B:120:ILE:HA | 8 | 0.11 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD11 | 7 | 0.11 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD12 | 7 | 0.11 |
| (1,2497) | 1:B:99:LEU:HB3 | 1:B:109:LEU:HD13 | 7 | 0.11 |
| (1,2495) | 1:B:99:LEU:HB2 | 1:B:163:LEU:HD11 | 6 | 0.11 |
| (1,2495) | 1:B:99:LEU:HB2 | 1:B:163:LEU:HD12 | 6 | 0.11 |
| (1,2495) | 1:B:99:LEU:HB2 | 1:B:163:LEU:HD13 | 6 | 0.11 |
| (1,2495) | 1:B:99:LEU:HB2 | 1:B:163:LEU:HD21 | 6 | 0.11 |
| (1,2495) | 1:B:99:LEU:HB2 | 1:B:163:LEU:HD22 | 6 | 0.11 |
| (1,2495) | 1:B:99:LEU:HB2 | 1:B:163:LEU:HD23 | 6 | 0.11 |
| (1,2457) | 1:B:98:SER:HA | 1:B:162:THR:HG21 | 9 | 0.11 |
| (1,2457) | 1:B:98:SER:HA | 1:B:162:THR:HG22 | 9 | 0.11 |
| (1,2457) | 1:B:98:SER:HA | 1:B:162:THR:HG23 | 9 | 0.11 |
| (1,2442) | 1:B:97:VAL:HG21 | 1:B:166:GLU:HA | 4 | 0.11 |
| (1,2442) | 1:B:97:VAL:HG22 | 1:B:166:GLU:HA | 4 | 0.11 |
| (1,2442) | 1:B:97:VAL:HG23 | 1:B:166:GLU:HA | 4 | 0.11 |
| (1,2442) | 1:B:97:VAL:HG21 | 1:B:166:GLU:HA | 8 | 0.11 |
| (1,2442) | 1:B:97:VAL:HG22 | 1:B:166:GLU:HA | 8 | 0.11 |
| (1,2442) | 1:B:97:VAL:HG23 | 1:B:166:GLU:HA | 8 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD1 | 1 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD2 | 1 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD1 | 1 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD2 | 1 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD1 | 1 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD2 | 1 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD1 | 3 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG11 | 1:B:142:TYR:HD2 | 3 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD1 | 3 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG12 | 1:B:142:TYR:HD2 | 3 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD1 | 3 | 0.11 |
| (1,2422) | 1:B:97:VAL:HG13 | 1:B:142:TYR:HD2 | 3 | 0.11 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG21 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG22 | 6 | 0.11 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG23 | 6 | 0.11 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG21 | 9 | 0.11 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG22 | 9 | 0.11 |
| (1,2413) | 1:B:97:VAL:HB | 1:B:165:VAL:HG23 | 9 | 0.11 |
| (1,2382) | 1:B:96:ARG:HB3 | 1:B:166:GLU:HA | 5 | 0.11 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG3 | 2 | 0.11 |
| (1,2378) | 1:B:96:ARG:HB2 | 1:B:166:GLU:HG2 | 2 | 0.11 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG21 | 4 | 0.11 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG22 | 4 | 0.11 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG23 | 4 | 0.11 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG21 | 7 | 0.11 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG22 | 7 | 0.11 |
| (1,2369) | 1:B:96:ARG:HA | 1:B:165:VAL:HG23 | 7 | 0.11 |
| (1,236) | 1:A:99:LEU:HD11 | 1:A:164:THR:HA | 3 | 0.11 |
| (1,236) | 1:A:99:LEU:HD12 | 1:A:164:THR:HA | 3 | 0.11 |
| (1,236) | 1:A:99:LEU:HD13 | 1:A:164:THR:HA | 3 | 0.11 |
| (1,2307) | 1:B:94:ARG:HA | 1:B:94:ARG:HD2 | 6 | 0.11 |
| (1,2307) | 1:B:94:ARG:HA | 1:B:94:ARG:HD3 | 6 | 0.11 |
| (1,2291) | 1:B:91:THR:HA | 1:B:91:THR:HB | 8 | 0.11 |
| (1,2244) | 1:B:136:ARG:HG2 | 1:A:138:PHE:HA | 8 | 0.11 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 2 | 0.11 |
| (1,2243) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 2 | 0.11 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 2 | 0.11 |
| (1,2243) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 2 | 0.11 |
| (1,2213) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 7 | 0.11 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 4 | 0.11 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 4 | 0.11 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 4 | 0.11 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD11 | 9 | 0.11 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD12 | 9 | 0.11 |
| (1,216) | 1:A:99:LEU:HB3 | 1:A:109:LEU:HD13 | 9 | 0.11 |
| (1,2155) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD1 | 2 | 0.11 |
| (1,2155) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD2 | 2 | 0.11 |
| (1,2112) | 1:B:136:ARG:HG2 | 1:A:138:PHE:HA | 8 | 0.11 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD1 | 2 | 0.11 |
| (1,2111) | 1:B:136:ARG:HB2 | 1:A:138:PHE:HD2 | 2 | 0.11 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD1 | 2 | 0.11 |
| (1,2111) | 1:B:136:ARG:HB3 | 1:A:138:PHE:HD2 | 2 | 0.11 |
| (1,2081) | 1:A:134:ILE:HA | 1:B:140:ARG:HD3 | 7 | 0.11 |
| (1,2023) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD1 | 2 | 0.11 |
| (1,2023) | 1:A:131:HIS:HB2 | 1:B:142:TYR:HD2 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1982) | 1:A:167:ALA:H | 1:A:166:GLU:HB3 | 10 | 0.11 |
| (1,1958) | 1:A:165:VAL:H | 1:A:166:GLU:HB3 | 7 | 0.11 |
| (1,1950) | 1:A:165:VAL:H | 1:A:96:ARG:HB2 | 2 | 0.11 |
| (1,1950) | 1:A:165:VAL:H | 1:A:96:ARG:HB3 | 2 | 0.11 |
| (1,1909) | 1:A:161:GLY:H | 1:A:160:GLU:HB3 | 2 | 0.11 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD11 | 10 | 0.11 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD12 | 10 | 0.11 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD13 | 10 | 0.11 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD21 | 10 | 0.11 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD22 | 10 | 0.11 |
| (1,1890) | 1:A:158:SER:H | 1:A:163:LEU:HD23 | 10 | 0.11 |
| (1,1888) | 1:A:158:SER:H | 1:A:162:THR:H | 1 | 0.11 |
| (1,1870) | 1:A:157:LEU:H | 1:A:157:LEU:HB3 | 9 | 0.11 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG11 | 9 | 0.11 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG12 | 9 | 0.11 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG13 | 9 | 0.11 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG21 | 9 | 0.11 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG22 | 9 | 0.11 |
| (1,1865) | 1:A:156:SER:H | 1:A:165:VAL:HG23 | 9 | 0.11 |
| (1,186) | 1:A:98:SER:HB2 | 1:A:164:THR:HA | 10 | 0.11 |
| (1,1849) | 1:A:155:SER:H | 1:A:156:SER:HA | 3 | 0.11 |
| (1,1816) | 1:A:153:VAL:H | 1:A:149:ASP:HB2 | 7 | 0.11 |
| (1,1805) | 1:A:152:GLN:HE21 | 1:A:170:PRO:HD2 | 10 | 0.11 |
| (1,1805) | 1:A:152:GLN:HE21 | 1:A:170:PRO:HD3 | 10 | 0.11 |
| (1,1803) | 1:A:152:GLN:HE21 | 1:A:168:PRO:HD2 | 4 | 0.11 |
| (1,1784) | 1:A:152:GLN:H | 1:A:149:ASP:HB3 | 6 | 0.11 |
| (1,1762) | 1:A:149:ASP:H | 1:A:152:GLN:HB2 | 7 | 0.11 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 2 | 0.11 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 2 | 0.11 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 2 | 0.11 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG11 | 7 | 0.11 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG12 | 7 | 0.11 |
| (1,1730) | 1:A:144:LEU:H | 1:A:148:VAL:HG13 | 7 | 0.11 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 1 | 0.11 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 1 | 0.11 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 1 | 0.11 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD11 | 2 | 0.11 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD12 | 2 | 0.11 |
| (1,1726) | 1:A:144:LEU:H | 1:A:144:LEU:HD13 | 2 | 0.11 |
| (1,1668) | 1:A:135:SER:H | 1:A:135:SER:HB3 | 5 | 0.11 |
| (1,1637) | 1:A:131:HIS:H | 1:A:130:GLU:HG2 | 8 | 0.11 |
| (1,1637) | 1:A:131:HIS:H | 1:A:130:GLU:HG3 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1636) | 1:A:131:HIS:H | 1:A:130:GLU:HB2 | 9 | 0.11 |
| (1,1636) | 1:A:131:HIS:H | 1:A:130:GLU:HB3 | 9 | 0.11 |
| (1,1627) | 1:A:129:ASP:H | 1:A:132:GLY:H | 9 | 0.11 |
| (1,1622) | 1:A:129:ASP:H | 1:A:129:ASP:HB3 | 8 | 0.11 |
| (1,1616) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HG2 | 3 | 0.11 |
| (1,1613) | 1:A:128:GLN:HE21 | 1:A:128:GLN:HA | 6 | 0.11 |
| (1,1611) | 1:A:128:GLN:HE22 | 1:A:128:GLN:H | 1 | 0.11 |
| (1,161) | 1:A:97:VAL:HG21 | 1:A:166:GLU:HA | 4 | 0.11 |
| (1,161) | 1:A:97:VAL:HG22 | 1:A:166:GLU:HA | 4 | 0.11 |
| (1,161) | 1:A:97:VAL:HG23 | 1:A:166:GLU:HA | 4 | 0.11 |
| (1,1600) | 1:A:128:GLN:H | 1:A:127:ARG:HD2 | 5 | 0.11 |
| (1,1598) | 1:A:128:GLN:H | 1:A:127:ARG:HG2 | 6 | 0.11 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD1 | 6 | 0.11 |
| (1,1596) | 1:A:127:ARG:H | 1:A:133:TYR:HD2 | 6 | 0.11 |
| (1,1591) | 1:A:126:GLU:H | 1:A:135:SER:HB2 | 1 | 0.11 |
| (1,1591) | 1:A:126:GLU:H | 1:A:135:SER:HB3 | 1 | 0.11 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB2 | 1 | 0.11 |
| (1,1586) | 1:A:126:GLU:H | 1:A:125:GLU:HB3 | 1 | 0.11 |
| (1,1581) | 1:A:125:GLU:H | 1:A:108:GLU:HG3 | 1 | 0.11 |
| (1,1580) | 1:A:125:GLU:H | 1:A:108:GLU:HG2 | 8 | 0.11 |
| (1,1576) | 1:A:124:HIS:H | 1:A:136:ARG:HA | 1 | 0.11 |
| (1,1576) | 1:A:124:HIS:H | 1:A:136:ARG:HA | 8 | 0.11 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD11 | 7 | 0.11 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD12 | 7 | 0.11 |
| (1,1568) | 1:A:123:LYS:H | 1:A:109:LEU:HD13 | 7 | 0.11 |
| (1,1567) | 1:A:123:LYS:H | 1:A:109:LEU:HG | 9 | 0.11 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB1 | 4 | 0.11 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB2 | 4 | 0.11 |
| (1,1563) | 1:A:123:LYS:H | 1:A:105:ALA:HB3 | 4 | 0.11 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG21 | 3 | 0.11 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG22 | 3 | 0.11 |
| (1,1556) | 1:A:121:THR:H | 1:A:121:THR:HG23 | 3 | 0.11 |
| (1,1546) | 1:A:120:ILE:H | 1:A:142:TYR:H | 9 | 0.11 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD11 | 10 | 0.11 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD12 | 10 | 0.11 |
| (1,1540) | 1:A:120:ILE:H | 1:A:120:ILE:HD13 | 10 | 0.11 |
| (1,1505) | 1:A:117:VAL:H | 1:A:117:VAL:HG21 | 9 | 0.11 |
| (1,1505) | 1:A:117:VAL:H | 1:A:117:VAL:HG22 | 9 | 0.11 |
| (1,1505) | 1:A:117:VAL:H | 1:A:117:VAL:HG23 | 9 | 0.11 |
| (1,1505) | 1:A:117:VAL:H | 1:A:117:VAL:HG11 | 9 | 0.11 |
| (1,1505) | 1:A:117:VAL:H | 1:A:117:VAL:HG12 | 9 | 0.11 |
| (1,1505) | 1:A:117:VAL:H | 1:A:117:VAL:HG13 | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1474) | 1:A:113:THR:H | 1:A:118:VAL:HG11 | 4 | 0.11 |
| (1,1474) | 1:A:113:THR:H | 1:A:118:VAL:HG12 | 4 | 0.11 |
| (1,1474) | 1:A:113:THR:H | 1:A:118:VAL:HG13 | 4 | 0.11 |
| (1,1474) | 1:A:113:THR:H | 1:A:118:VAL:HG21 | 4 | 0.11 |
| (1,1474) | 1:A:113:THR:H | 1:A:118:VAL:HG22 | 4 | 0.11 |
| (1,1474) | 1:A:113:THR:H | 1:A:118:VAL:HG23 | 4 | 0.11 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG21 | 5 | 0.11 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG22 | 5 | 0.11 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG23 | 5 | 0.11 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG11 | 5 | 0.11 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG12 | 5 | 0.11 |
| (1,1456) | 1:A:112:LYS:H | 1:A:111:VAL:HG13 | 5 | 0.11 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD11 | 8 | 0.11 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD12 | 8 | 0.11 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD13 | 8 | 0.11 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD11 | 10 | 0.11 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD12 | 10 | 0.11 |
| (1,1439) | 1:A:110:THR:H | 1:A:120:ILE:HD13 | 10 | 0.11 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD1 | 1 | 0.11 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD2 | 1 | 0.11 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD1 | 1 | 0.11 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD2 | 1 | 0.11 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD1 | 1 | 0.11 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD2 | 1 | 0.11 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD1 | 4 | 0.11 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD2 | 4 | 0.11 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD1 | 4 | 0.11 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD2 | 4 | 0.11 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD1 | 4 | 0.11 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD2 | 4 | 0.11 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD1 | 5 | 0.11 |
| (1,141) | 1:A:97:VAL:HG11 | 1:A:142:TYR:HD2 | 5 | 0.11 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD1 | 5 | 0.11 |
| (1,141) | 1:A:97:VAL:HG12 | 1:A:142:TYR:HD2 | 5 | 0.11 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD1 | 5 | 0.11 |
| (1,141) | 1:A:97:VAL:HG13 | 1:A:142:TYR:HD2 | 5 | 0.11 |
| (1,1391) | 1:A:105:ALA:H | 1:A:108:GLU:HB3 | 2 | 0.11 |
| (1,1389) | 1:A:105:ALA:H | 1:A:106:PRO:HD3 | 4 | 0.11 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD21 | 7 | 0.11 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD22 | 7 | 0.11 |
| (1,1384) | 1:A:103:HIS:H | 1:A:109:LEU:HD23 | 7 | 0.11 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG11 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG12 | 5 | 0.11 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG13 | 5 | 0.11 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG21 | 5 | 0.11 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG22 | 5 | 0.11 |
| (1,1357) | 1:A:99:LEU:H | 1:A:101:VAL:HG23 | 5 | 0.11 |
| (1,1345) | 1:A:97:VAL:H | 1:A:165:VAL:H | 2 | 0.11 |
| (1,1324) | 1:A:94:ARG:H | 1:A:94:ARG:HG2 | 7 | 0.11 |
| (1,1324) | 1:A:94:ARG:H | 1:A:94:ARG:HG3 | 7 | 0.11 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG21 | 8 | 0.11 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG22 | 8 | 0.11 |
| (1,132) | 1:A:97:VAL:HB | 1:A:165:VAL:HG23 | 8 | 0.11 |
| (1,1311) | 1:A:170:PRO:HB2 | 1:A:170:PRO:HG2 | 5 | 0.11 |
| (1,1311) | 1:A:170:PRO:HB2 | 1:A:170:PRO:HG2 | 6 | 0.11 |
| (1,1311) | 1:A:170:PRO:HB2 | 1:A:170:PRO:HG2 | 8 | 0.11 |
| (1,1282) | 1:A:168:PRO:HB3 | 1:A:169:MET:HA | 5 | 0.11 |
| (1,1282) | 1:A:168:PRO:HB3 | 1:A:169:MET:HA | 10 | 0.11 |
| (1,1276) | 1:A:168:PRO:HA | 1:A:169:MET:HG2 | 1 | 0.11 |
| (1,1260) | 1:A:166:GLU:HG3 | 1:A:168:PRO:HD2 | 5 | 0.11 |
| (1,1260) | 1:A:166:GLU:HG2 | 1:A:168:PRO:HD2 | 5 | 0.11 |
| (1,1260) | 1:A:166:GLU:HG2 | 1:A:168:PRO:HD3 | 5 | 0.11 |
| (1,1260) | 1:A:166:GLU:HG3 | 1:A:168:PRO:HD3 | 5 | 0.11 |
| (1,1248) | 1:A:165:VAL:HG21 | 1:A:167:ALA:HA | 2 | 0.11 |
| (1,1248) | 1:A:165:VAL:HG22 | 1:A:167:ALA:HA | 2 | 0.11 |
| (1,1248) | 1:A:165:VAL:HG23 | 1:A:167:ALA:HA | 2 | 0.11 |
| (1,1192) | 1:A:158:SER:HB2 | 1:A:162:THR:HB | 8 | 0.11 |
| (1,1172) | 1:A:157:LEU:HD11 | 1:A:163:LEU:HB2 | 10 | 0.11 |
| (1,1172) | 1:A:157:LEU:HD12 | 1:A:163:LEU:HB2 | 10 | 0.11 |
| (1,1172) | 1:A:157:LEU:HD13 | 1:A:163:LEU:HB2 | 10 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD11 | 2 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD12 | 2 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD13 | 2 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD21 | 2 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD22 | 2 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD23 | 2 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD11 | 3 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD12 | 3 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD13 | 3 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD21 | 3 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD22 | 3 | 0.11 |
| (1,1165) | 1:A:157:LEU:HG | 1:A:163:LEU:HD23 | 3 | 0.11 |
| (1,1155) | 1:A:157:LEU:HB2 | 1:A:163:LEU:HA | 10 | 0.11 |
| (1,1149) | 1:A:157:LEU:HA | 1:A:163:LEU:HB3 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD11 | 1 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD12 | 1 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD13 | 1 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD11 | 2 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD12 | 2 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD13 | 2 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD11 | 8 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD12 | 8 | 0.11 |
| (1,1144) | 1:A:157:LEU:HA | 1:A:157:LEU:HD13 | 8 | 0.11 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD11 | 4 | 0.11 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD12 | 4 | 0.11 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD13 | 4 | 0.11 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD21 | 4 | 0.11 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD22 | 4 | 0.11 |
| (1,1106) | 1:A:155:SER:HA | 1:A:163:LEU:HD23 | 4 | 0.11 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB1 | 1 | 0.11 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB2 | 1 | 0.11 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB3 | 1 | 0.11 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB1 | 10 | 0.11 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB2 | 10 | 0.11 |
| (1,11) | 1:A:91:THR:HB | 1:A:92:ALA:HB3 | 10 | 0.11 |
| (1,1027) | 1:A:149:ASP:HA | 1:A:150:PRO:HG3 | 6 | 0.11 |
| (1,102) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HB3 | 4 | 0.11 |
| (1,101) | 1:A:96:ARG:HB3 | 1:A:166:GLU:HA | 5 | 0.11 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG21 | 3 | 0.11 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG22 | 3 | 0.11 |
| (1,100) | 1:A:96:ARG:HB3 | 1:A:164:THR:HG23 | 3 | 0.11 |

# 10 Dihedral-angle violation analysis (i)

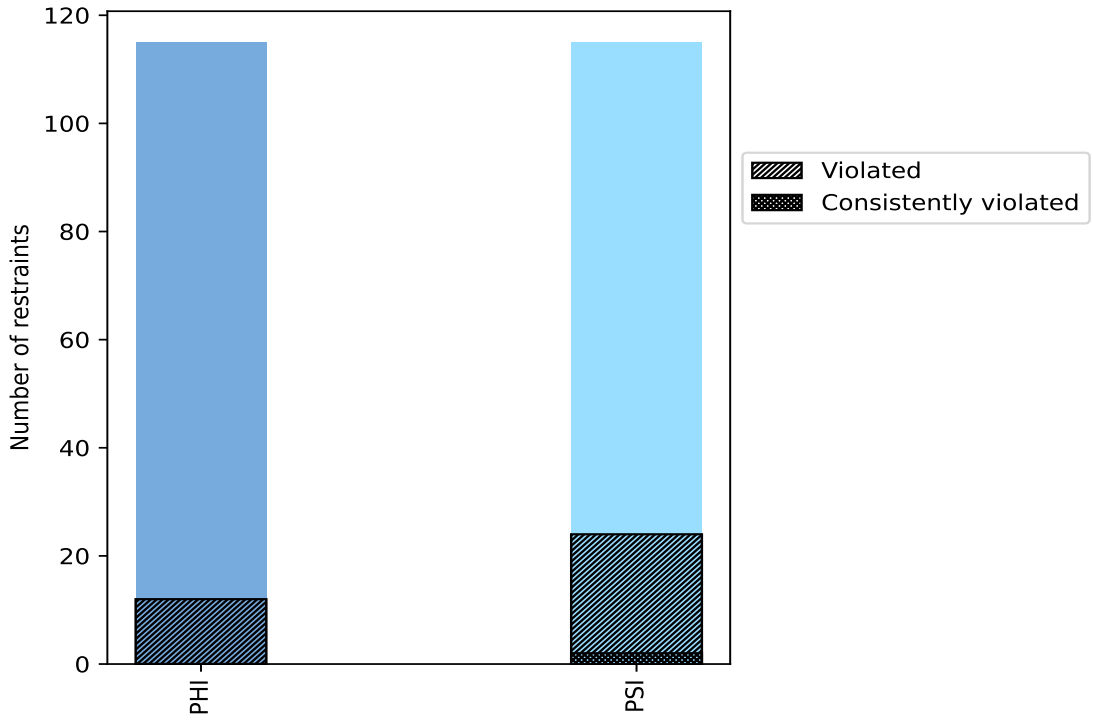
## 10.1 Summary of dihedral-angle violations (i)

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

| Angle type | Count | %[1] | Violated[3] | | | Consistently Violated[4] | | |
|---|---|---|---|---|---|---|---|---|
| | | | Count | %[2] | %[1] | Count | %[2] | %[1] |
| PHI | 115 | 50.0 | 12 | 10.4 | 5.2 | 0 | 0.0 | 0.0 |
| PSI | 115 | 50.0 | 24 | 20.9 | 10.4 | 2 | 1.7 | 0.9 |
| Total | 230 | 100.0 | 36 | 15.7 | 15.7 | 2 | 0.9 | 0.9 |

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

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



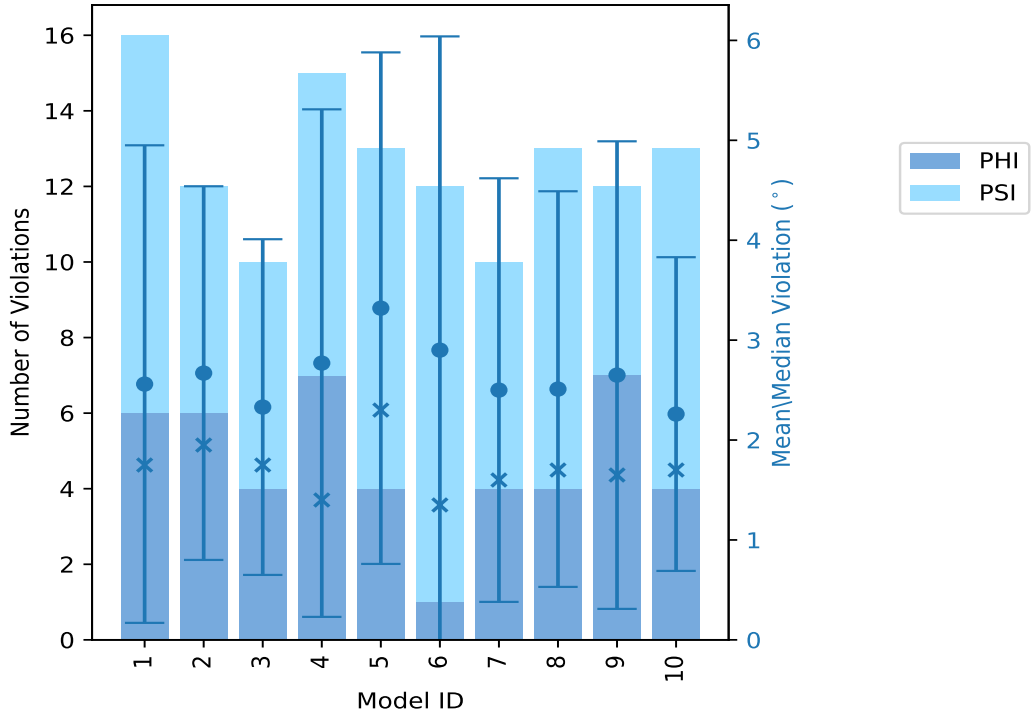

Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model (i)

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|---|---|---|---|---|---|---|---|
| | PHI | PSI | Total | | | | |
| 1 | 6 | 10 | 16 | 2.56 | 9.2 | 2.39 | 1.75 |
| 2 | 6 | 6 | 12 | 2.67 | 7.8 | 1.87 | 1.95 |
| 3 | 4 | 6 | 10 | 2.33 | 7.0 | 1.68 | 1.75 |
| 4 | 7 | 8 | 15 | 2.77 | 9.0 | 2.54 | 1.4 |
| 5 | 4 | 9 | 13 | 3.32 | 9.8 | 2.56 | 2.3 |
| 6 | 1 | 11 | 12 | 2.9 | 10.0 | 3.14 | 1.35 |
| 7 | 4 | 6 | 10 | 2.5 | 7.7 | 2.12 | 1.6 |
| 8 | 4 | 9 | 13 | 2.51 | 7.5 | 1.98 | 1.7 |
| 9 | 7 | 5 | 12 | 2.65 | 8.7 | 2.34 | 1.65 |
| 10 | 4 | 9 | 13 | 2.26 | 7.3 | 1.57 | 1.7 |

### 10.2.1 Bar graph : Dihedral violation statistics for each model (i)




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

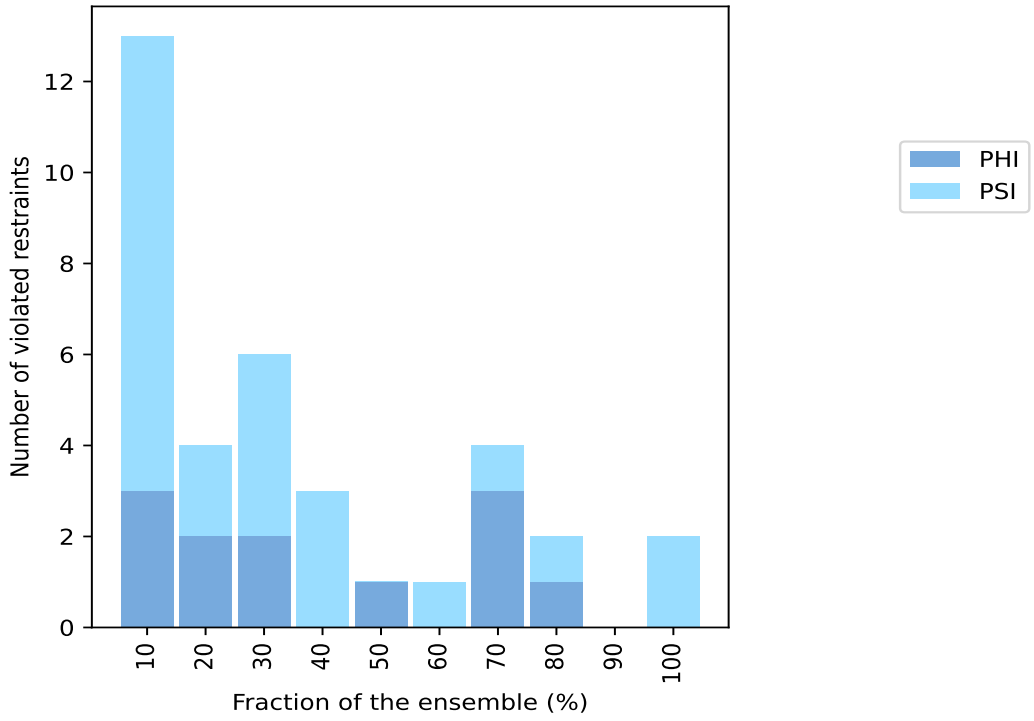
## 10.3 Dihedral-angle violation statistics for the ensemble (i)

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

| Number of violated restraints | | | Fraction of the ensemble | |
|---|---|---|---|---|
| PHI | PSI | Total | Count[1] | % |
| 3 | 10 | 13 | 1 | 10.0 |
| 2 | 2 | 4 | 2 | 20.0 |
| 2 | 4 | 6 | 3 | 30.0 |
| 0 | 3 | 3 | 4 | 40.0 |
| 1 | 0 | 1 | 5 | 50.0 |
| 0 | 1 | 1 | 6 | 60.0 |
| 3 | 1 | 4 | 7 | 70.0 |
| 1 | 1 | 2 | 8 | 80.0 |
| 0 | 0 | 0 | 9 | 90.0 |
| 0 | 2 | 2 | 10 | 100.0 |

[1] Number of models with violations

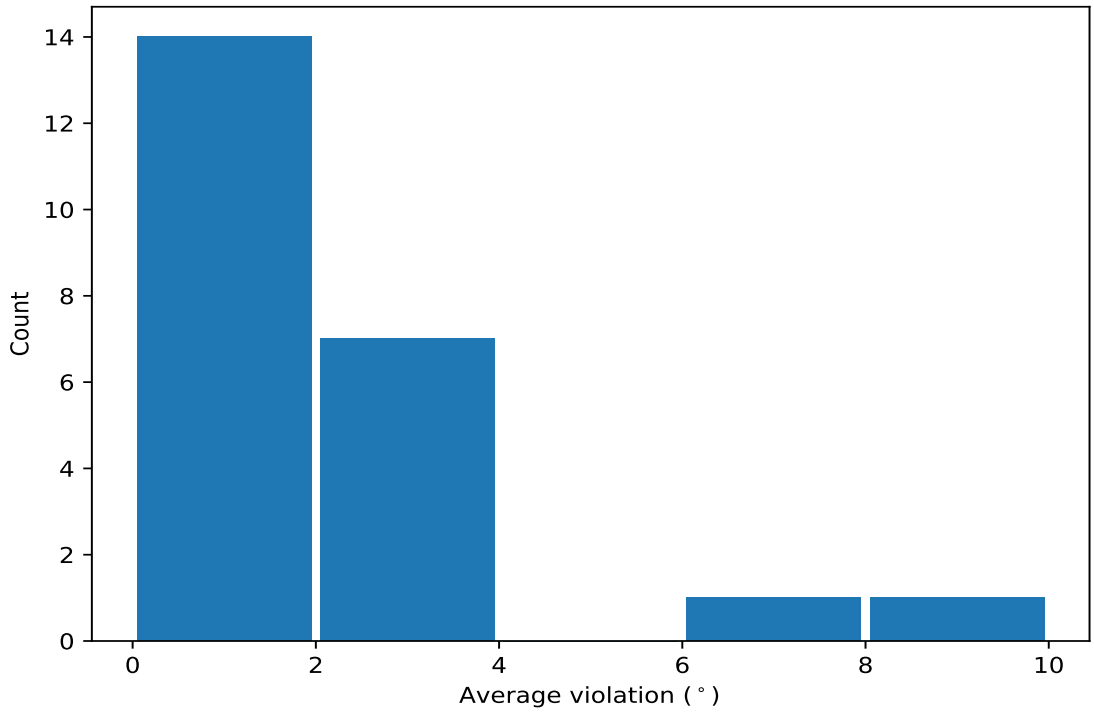
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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

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

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




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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models[1] | Mean | SD[2] | Median |
|---|---|---|---|---|---|---|---|---|
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 10 | 8.09 | 0.98 | 7.95 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 10 | 6.86 | 2.24 | 7.1 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 8 | 2.2 | 0.49 | 2.3 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 8 | 1.81 | 0.49 | 1.85 |
| (1,58) | 1:A:132:GLY:C | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 7 | 2.5 | 1.22 | 1.9 |
| (1,87) | 1:A:150:PRO:C | 1:A:151:THR:N | 1:A:151:THR:CA | 1:A:151:THR:C | 7 | 1.64 | 0.45 | 1.6 |
| (1,16) | 1:A:107:ASP:N | 1:A:107:ASP:CA | 1:A:107:ASP:C | 1:A:108:GLU:N | 7 | 1.59 | 0.3 | 1.7 |
| (1,146) | 1:B:116:GLY:C | 1:B:117:VAL:N | 1:B:117:VAL:CA | 1:B:117:VAL:C | 7 | 1.46 | 0.13 | 1.5 |
| (1,132) | 1:B:107:ASP:N | 1:B:107:ASP:CA | 1:B:107:ASP:C | 1:B:108:GLU:N | 6 | 1.45 | 0.35 | 1.3 |
| (1,30) | 1:A:116:GLY:C | 1:A:117:VAL:N | 1:A:117:VAL:CA | 1:A:117:VAL:C | 5 | 2.0 | 0.18 | 1.9 |
| (1,163) | 1:B:126:GLU:N | 1:B:126:GLU:CA | 1:B:126:GLU:C | 1:B:127:ARG:N | 4 | 2.15 | 0.62 | 1.95 |
| (1,144) | 1:B:115:ASP:N | 1:B:115:ASP:CA | 1:B:115:ASP:C | 1:B:116:GLY:N | 4 | 2.0 | 0.73 | 1.85 |
| (1,28) | 1:A:115:ASP:N | 1:A:115:ASP:CA | 1:A:115:ASP:C | 1:A:116:GLY:N | 4 | 1.5 | 0.21 | 1.5 |

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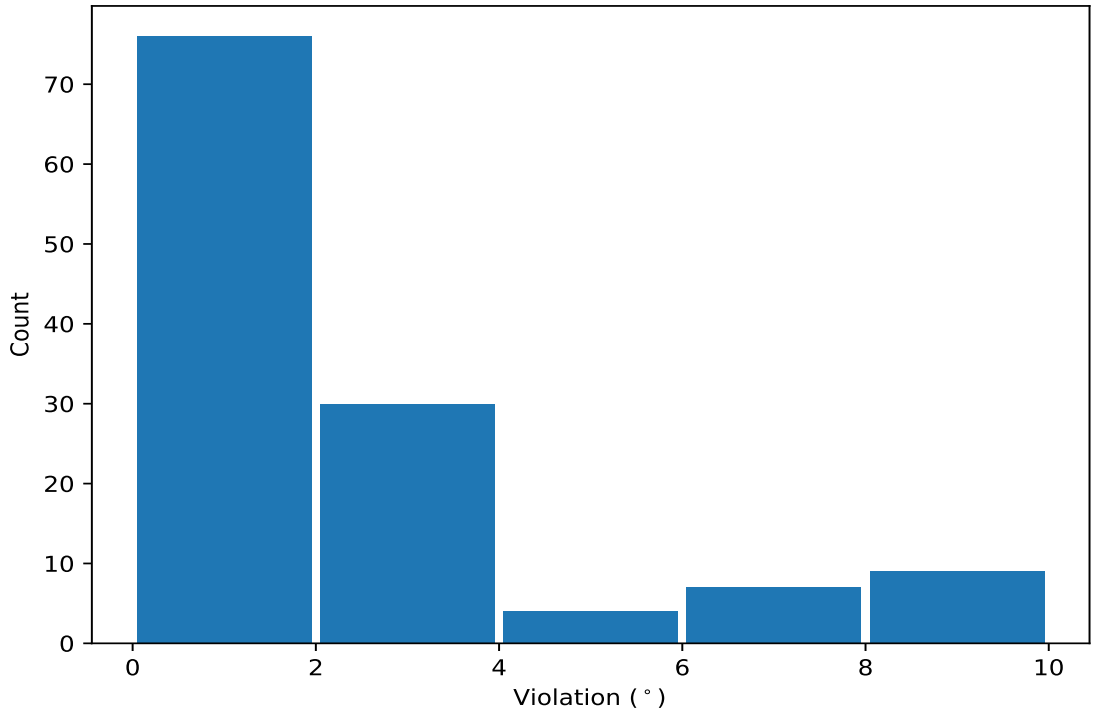
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models[1] | Mean | SD[2] | Median |
|---|---|---|---|---|---|---|---|---|
| (1,57) | 1:A:131:HIS:N | 1:A:131:HIS:CA | 1:A:131:HIS:C | 1:A:132:GLY:N | 3 | 2.2 | 1.02 | 1.8 |
| (1,115) | 1:A:168:PRO:N | 1:A:168:PRO:CA | 1:A:168:PRO:C | 1:A:169:MET:N | 3 | 2.07 | 1.16 | 1.3 |
| (1,47) | 1:A:126:GLU:N | 1:A:126:GLU:CA | 1:A:126:GLU:C | 1:A:127:ARG:N | 3 | 1.57 | 0.52 | 1.2 |
| (1,203) | 1:B:150:PRO:C | 1:B:151:THR:N | 1:B:151:THR:CA | 1:B:151:THR:C | 3 | 1.37 | 0.21 | 1.4 |
| (1,221) | 1:B:161:GLY:N | 1:B:161:GLY:CA | 1:B:161:GLY:C | 1:B:162:THR:N | 3 | 1.3 | 0.22 | 1.2 |
| (1,201) | 1:B:149:ASP:C | 1:B:150:PRO:N | 1:B:150:PRO:CA | 1:B:150:PRO:C | 3 | 1.2 | 0.14 | 1.1 |
| (1,174) | 1:B:132:GLY:C | 1:B:133:TYR:N | 1:B:133:TYR:CA | 1:B:133:TYR:C | 2 | 1.8 | 0.2 | 1.8 |
| (1,105) | 1:A:161:GLY:N | 1:A:161:GLY:CA | 1:A:161:GLY:C | 1:A:162:THR:N | 2 | 1.6 | 0.1 | 1.6 |
| (1,42) | 1:A:122:GLY:C | 1:A:123:LYS:N | 1:A:123:LYS:CA | 1:A:123:LYS:C | 2 | 1.2 | 0.1 | 1.2 |
| (1,79) | 1:A:143:THR:N | 1:A:143:THR:CA | 1:A:143:THR:C | 1:A:144:LEU:N | 2 | 1.1 | 0.0 | 1.1 |

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

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

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

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




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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 6 | 10.0 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 5 | 9.8 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 6 | 9.5 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 1 | 9.2 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 4 | 9.0 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 9 | 8.7 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 4 | 8.5 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 1 | 8.3 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 5 | 8.1 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 2 | 7.8 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 7 | 7.7 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 8 | 7.5 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 10 | 7.3 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 3 | 7.0 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 9 | 6.7 |
| (1,81) | 1:A:144:LEU:N | 1:A:144:LEU:CA | 1:A:144:LEU:C | 1:A:145:PRO:N | 8 | 6.6 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 2 | 5.5 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 7 | 5.5 |
| (1,58) | 1:A:132:GLY:C | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 5 | 4.5 |
| (1,58) | 1:A:132:GLY:C | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 4 | 4.3 |
| (1,115) | 1:A:168:PRO:N | 1:A:168:PRO:CA | 1:A:168:PRO:C | 1:A:169:MET:N | 4 | 3.7 |
| (1,57) | 1:A:131:HIS:N | 1:A:131:HIS:CA | 1:A:131:HIS:C | 1:A:132:GLY:N | 6 | 3.6 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 3 | 3.5 |
| (1,197) | 1:B:144:LEU:N | 1:B:144:LEU:CA | 1:B:144:LEU:C | 1:B:145:PRO:N | 10 | 3.3 |
| (1,163) | 1:B:126:GLU:N | 1:B:126:GLU:CA | 1:B:126:GLU:C | 1:B:127:ARG:N | 1 | 3.1 |
| (1,144) | 1:B:115:ASP:N | 1:B:115:ASP:CA | 1:B:115:ASP:C | 1:B:116:GLY:N | 5 | 3.1 |
| (1,158) | 1:B:122:GLY:C | 1:B:123:LYS:N | 1:B:123:LYS:CA | 1:B:123:LYS:C | 4 | 2.8 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 5 | 2.7 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 10 | 2.7 |
| (1,87) | 1:A:150:PRO:C | 1:A:151:THR:N | 1:A:151:THR:CA | 1:A:151:THR:C | 9 | 2.5 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 8 | 2.5 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 2 | 2.5 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 9 | 2.4 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 5 | 2.4 |
| (1,47) | 1:A:126:GLU:N | 1:A:126:GLU:CA | 1:A:126:GLU:C | 1:A:127:ARG:N | 10 | 2.3 |
| (1,30) | 1:A:116:GLY:C | 1:A:117:VAL:N | 1:A:117:VAL:CA | 1:A:117:VAL:C | 5 | 2.3 |
| (1,163) | 1:B:126:GLU:N | 1:B:126:GLU:CA | 1:B:126:GLU:C | 1:B:127:ARG:N | 5 | 2.3 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 2 | 2.2 |
| (1,59) | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 1:A:134:ILE:N | 4 | 2.2 |
| (1,144) | 1:B:115:ASP:N | 1:B:115:ASP:CA | 1:B:115:ASP:C | 1:B:116:GLY:N | 2 | 2.2 |
| (1,132) | 1:B:107:ASP:N | 1:B:107:ASP:CA | 1:B:107:ASP:C | 1:B:108:GLU:N | 5 | 2.2 |
| (1,58) | 1:A:132:GLY:C | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 3 | 2.1 |
| (1,30) | 1:A:116:GLY:C | 1:A:117:VAL:N | 1:A:117:VAL:CA | 1:A:117:VAL:C | 8 | 2.1 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 8 | 2.1 |
| (1,87) | 1:A:150:PRO:C | 1:A:151:THR:N | 1:A:151:THR:CA | 1:A:151:THR:C | 2 | 2.0 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 1 | 2.0 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 3 | 2.0 |
| (1,44) | 1:A:123:LYS:C | 1:A:124:HIS:N | 1:A:124:HIS:CA | 1:A:124:HIS:C | 1 | 2.0 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 1 | 2.0 |
| (1,174) | 1:B:132:GLY:C | 1:B:133:TYR:N | 1:B:133:TYR:CA | 1:B:133:TYR:C | 9 | 2.0 |
| (1,58) | 1:A:132:GLY:C | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 7 | 1.9 |
| (1,30) | 1:A:116:GLY:C | 1:A:117:VAL:N | 1:A:117:VAL:CA | 1:A:117:VAL:C | 2 | 1.9 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,30) | 1:A:116:GLY:C | 1:A:117:VAL:N | 1:A:117:VAL:CA | 1:A:117:VAL:C | 10 | 1.9 |
| (1,16) | 1:A:107:ASP:N | 1:A:107:ASP:CA | 1:A:107:ASP:C | 1:A:108:GLU:N | 1 | 1.9 |
| (1,16) | 1:A:107:ASP:N | 1:A:107:ASP:CA | 1:A:107:ASP:C | 1:A:108:GLU:N | 2 | 1.9 |
| (1,57) | 1:A:131:HIS:N | 1:A:131:HIS:CA | 1:A:131:HIS:C | 1:A:132:GLY:N | 10 | 1.8 |
| (1,45) | 1:A:124:HIS:N | 1:A:124:HIS:CA | 1:A:124:HIS:C | 1:A:125:GLU:N | 1 | 1.8 |
| (1,30) | 1:A:116:GLY:C | 1:A:117:VAL:N | 1:A:117:VAL:CA | 1:A:117:VAL:C | 3 | 1.8 |
| (1,28) | 1:A:115:ASP:N | 1:A:115:ASP:CA | 1:A:115:ASP:C | 1:A:116:GLY:N | 9 | 1.8 |
| (1,16) | 1:A:107:ASP:N | 1:A:107:ASP:CA | 1:A:107:ASP:C | 1:A:108:GLU:N | 8 | 1.8 |
| (1,87) | 1:A:150:PRO:C | 1:A:151:THR:N | 1:A:151:THR:CA | 1:A:151:THR:C | 8 | 1.7 |
| (1,58) | 1:A:132:GLY:C | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 1 | 1.7 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 3 | 1.7 |
| (1,16) | 1:A:107:ASP:N | 1:A:107:ASP:CA | 1:A:107:ASP:C | 1:A:108:GLU:N | 10 | 1.7 |
| (1,112) | 1:A:165:VAL:N | 1:A:165:VAL:CA | 1:A:165:VAL:C | 1:A:166:GLU:N | 6 | 1.7 |
| (1,105) | 1:A:161:GLY:N | 1:A:161:GLY:CA | 1:A:161:GLY:C | 1:A:162:THR:N | 10 | 1.7 |
| (1,87) | 1:A:150:PRO:C | 1:A:151:THR:N | 1:A:151:THR:CA | 1:A:151:THR:C | 7 | 1.6 |
| (1,58) | 1:A:132:GLY:C | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 2 | 1.6 |
| (1,221) | 1:B:161:GLY:N | 1:B:161:GLY:CA | 1:B:161:GLY:C | 1:B:162:THR:N | 7 | 1.6 |
| (1,203) | 1:B:150:PRO:C | 1:B:151:THR:N | 1:B:151:THR:CA | 1:B:151:THR:C | 2 | 1.6 |
| (1,174) | 1:B:132:GLY:C | 1:B:133:TYR:N | 1:B:133:TYR:CA | 1:B:133:TYR:C | 7 | 1.6 |
| (1,169) | 1:B:129:ASP:N | 1:B:129:ASP:CA | 1:B:129:ASP:C | 1:B:130:GLU:N | 8 | 1.6 |
| (1,163) | 1:B:126:GLU:N | 1:B:126:GLU:CA | 1:B:126:GLU:C | 1:B:127:ARG:N | 6 | 1.6 |
| (1,163) | 1:B:126:GLU:N | 1:B:126:GLU:CA | 1:B:126:GLU:C | 1:B:127:ARG:N | 8 | 1.6 |
| (1,146) | 1:B:116:GLY:C | 1:B:117:VAL:N | 1:B:117:VAL:CA | 1:B:117:VAL:C | 7 | 1.6 |
| (1,146) | 1:B:116:GLY:C | 1:B:117:VAL:N | 1:B:117:VAL:CA | 1:B:117:VAL:C | 10 | 1.6 |
| (1,28) | 1:A:115:ASP:N | 1:A:115:ASP:CA | 1:A:115:ASP:C | 1:A:116:GLY:N | 2 | 1.5 |
| (1,28) | 1:A:115:ASP:N | 1:A:115:ASP:CA | 1:A:115:ASP:C | 1:A:116:GLY:N | 8 | 1.5 |
| (1,172) | 1:B:130:GLU:C | 1:B:131:HIS:N | 1:B:131:HIS:CA | 1:B:131:HIS:C | 1 | 1.5 |
| (1,16) | 1:A:107:ASP:N | 1:A:107:ASP:CA | 1:A:107:ASP:C | 1:A:108:GLU:N | 5 | 1.5 |
| (1,146) | 1:B:116:GLY:C | 1:B:117:VAL:N | 1:B:117:VAL:CA | 1:B:117:VAL:C | 3 | 1.5 |
| (1,146) | 1:B:116:GLY:C | 1:B:117:VAL:N | 1:B:117:VAL:CA | 1:B:117:VAL:C | 4 | 1.5 |
| (1,144) | 1:B:115:ASP:N | 1:B:115:ASP:CA | 1:B:115:ASP:C | 1:B:116:GLY:N | 6 | 1.5 |
| (1,132) | 1:B:107:ASP:N | 1:B:107:ASP:CA | 1:B:107:ASP:C | 1:B:108:GLU:N | 9 | 1.5 |
| (1,105) | 1:A:161:GLY:N | 1:A:161:GLY:CA | 1:A:161:GLY:C | 1:A:162:THR:N | 5 | 1.5 |
| (1,87) | 1:A:150:PRO:C | 1:A:151:THR:N | 1:A:151:THR:CA | 1:A:151:THR:C | 5 | 1.4 |
| (1,58) | 1:A:132:GLY:C | 1:A:133:TYR:N | 1:A:133:TYR:CA | 1:A:133:TYR:C | 10 | 1.4 |
| (1,203) | 1:B:150:PRO:C | 1:B:151:THR:N | 1:B:151:THR:CA | 1:B:151:THR:C | 9 | 1.4 |
| (1,201) | 1:B:149:ASP:C | 1:B:150:PRO:N | 1:B:150:PRO:CA | 1:B:150:PRO:C | 4 | 1.4 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 10 | 1.4 |
| (1,146) | 1:B:116:GLY:C | 1:B:117:VAL:N | 1:B:117:VAL:CA | 1:B:117:VAL:C | 1 | 1.4 |
| (1,146) | 1:B:116:GLY:C | 1:B:117:VAL:N | 1:B:117:VAL:CA | 1:B:117:VAL:C | 9 | 1.4 |
| (1,132) | 1:B:107:ASP:N | 1:B:107:ASP:CA | 1:B:107:ASP:C | 1:B:108:GLU:N | 1 | 1.4 |
| (1,104) | 1:A:160:GLU:N | 1:A:160:GLU:CA | 1:A:160:GLU:C | 1:A:161:GLY:N | 3 | 1.4 |
| (1,42) | 1:A:122:GLY:C | 1:A:123:LYS:N | 1:A:123:LYS:CA | 1:A:123:LYS:C | 2 | 1.3 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 4 | 1.3 |
| (1,117) | 1:B:96:ARG:N | 1:B:96:ARG:CA | 1:B:96:ARG:C | 1:B:97:VAL:N | 1 | 1.3 |
| (1,115) | 1:A:168:PRO:N | 1:A:168:PRO:CA | 1:A:168:PRO:C | 1:A:169:MET:N | 5 | 1.3 |
| (1,87) | 1:A:150:PRO:C | 1:A:151:THR:N | 1:A:151:THR:CA | 1:A:151:THR:C | 4 | 1.2 |
| (1,57) | 1:A:131:HIS:N | 1:A:131:HIS:CA | 1:A:131:HIS:C | 1:A:132:GLY:N | 9 | 1.2 |
| (1,47) | 1:A:126:GLU:N | 1:A:126:GLU:CA | 1:A:126:GLU:C | 1:A:127:ARG:N | 6 | 1.2 |
| (1,47) | 1:A:126:GLU:N | 1:A:126:GLU:CA | 1:A:126:GLU:C | 1:A:127:ARG:N | 8 | 1.2 |
| (1,28) | 1:A:115:ASP:N | 1:A:115:ASP:CA | 1:A:115:ASP:C | 1:A:116:GLY:N | 1 | 1.2 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,221) | 1:B:161:GLY:N | 1:B:161:GLY:CA | 1:B:161:GLY:C | 1:B:162:THR:N | 6 | 1.2 |
| (1,16) | 1:A:107:ASP:N | 1:A:107:ASP:CA | 1:A:107:ASP:C | 1:A:108:GLU:N | 7 | 1.2 |
| (1,146) | 1:B:116:GLY:C | 1:B:117:VAL:N | 1:B:117:VAL:CA | 1:B:117:VAL:C | 8 | 1.2 |
| (1,144) | 1:B:115:ASP:N | 1:B:115:ASP:CA | 1:B:115:ASP:C | 1:B:116:GLY:N | 3 | 1.2 |
| (1,132) | 1:B:107:ASP:N | 1:B:107:ASP:CA | 1:B:107:ASP:C | 1:B:108:GLU:N | 4 | 1.2 |
| (1,132) | 1:B:107:ASP:N | 1:B:107:ASP:CA | 1:B:107:ASP:C | 1:B:108:GLU:N | 6 | 1.2 |
| (1,132) | 1:B:107:ASP:N | 1:B:107:ASP:CA | 1:B:107:ASP:C | 1:B:108:GLU:N | 8 | 1.2 |
| (1,115) | 1:A:168:PRO:N | 1:A:168:PRO:CA | 1:A:168:PRO:C | 1:A:169:MET:N | 10 | 1.2 |
| (1,10) | 1:A:102:ASN:N | 1:A:102:ASN:CA | 1:A:102:ASN:C | 1:A:103:HIS:N | 7 | 1.2 |
| (1,87) | 1:A:150:PRO:C | 1:A:151:THR:N | 1:A:151:THR:CA | 1:A:151:THR:C | 1 | 1.1 |
| (1,85) | 1:A:149:ASP:C | 1:A:150:PRO:N | 1:A:150:PRO:CA | 1:A:150:PRO:C | 4 | 1.1 |
| (1,79) | 1:A:143:THR:N | 1:A:143:THR:CA | 1:A:143:THR:C | 1:A:144:LEU:N | 1 | 1.1 |
| (1,79) | 1:A:143:THR:N | 1:A:143:THR:CA | 1:A:143:THR:C | 1:A:144:LEU:N | 10 | 1.1 |
| (1,42) | 1:A:122:GLY:C | 1:A:123:LYS:N | 1:A:123:LYS:CA | 1:A:123:LYS:C | 9 | 1.1 |
| (1,228) | 1:B:165:VAL:N | 1:B:165:VAL:CA | 1:B:165:VAL:C | 1:B:166:GLU:N | 3 | 1.1 |
| (1,221) | 1:B:161:GLY:N | 1:B:161:GLY:CA | 1:B:161:GLY:C | 1:B:162:THR:N | 4 | 1.1 |
| (1,203) | 1:B:150:PRO:C | 1:B:151:THR:N | 1:B:151:THR:CA | 1:B:151:THR:C | 4 | 1.1 |
| (1,201) | 1:B:149:ASP:C | 1:B:150:PRO:N | 1:B:150:PRO:CA | 1:B:150:PRO:C | 6 | 1.1 |
| (1,201) | 1:B:149:ASP:C | 1:B:150:PRO:N | 1:B:150:PRO:CA | 1:B:150:PRO:C | 9 | 1.1 |
| (1,193) | 1:B:142:TYR:N | 1:B:142:TYR:CA | 1:B:142:TYR:C | 1:B:143:THR:N | 6 | 1.1 |
| (1,173) | 1:B:131:HIS:N | 1:B:131:HIS:CA | 1:B:131:HIS:C | 1:B:132:GLY:N | 7 | 1.1 |
| (1,16) | 1:A:107:ASP:N | 1:A:107:ASP:CA | 1:A:107:ASP:C | 1:A:108:GLU:N | 4 | 1.1 |
| (1,1) | 1:A:96:ARG:N | 1:A:96:ARG:CA | 1:A:96:ARG:C | 1:A:97:VAL:N | 6 | 1.1 |