# Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2026 – 10:58 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 7KW9 / pdb_00007kw9 |
| BMRB ID | : | 30820 |
| Title | : | NMR Structure of a tRNA 2'-phosphotransferase from Runella slithyformis in complex with NAD+ |
| Authors | : | Alphonse, S.; Dantuluri, S.; Banerjee, A.; Shuman, S.; Ghose, R. |
| Deposited on | : | 2020-11-30 |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

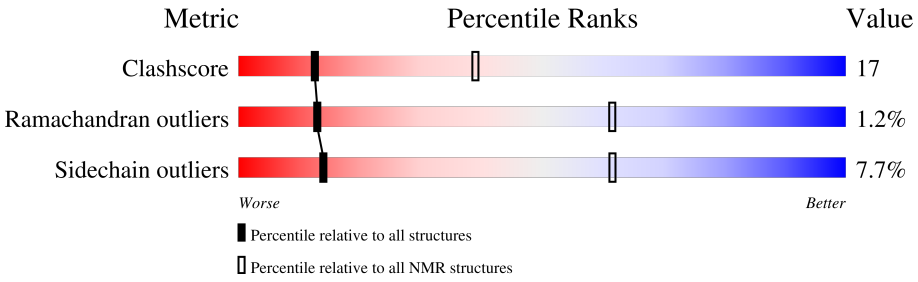
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 81%.

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




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 229148 | 14424 |
| Ramachandran outliers | 224038 | 12848 |
| Sidechain outliers | 223484 | 12823 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 178 | 63% 18% 6% • 12% |

# 2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:4-A:77 (74) | 0.53 | 9 |
| 2 | A:91-A:115, A:121-A:178 (83) | 0.75 | 19 |

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 4 clusters and 5 single-model clusters were found.

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

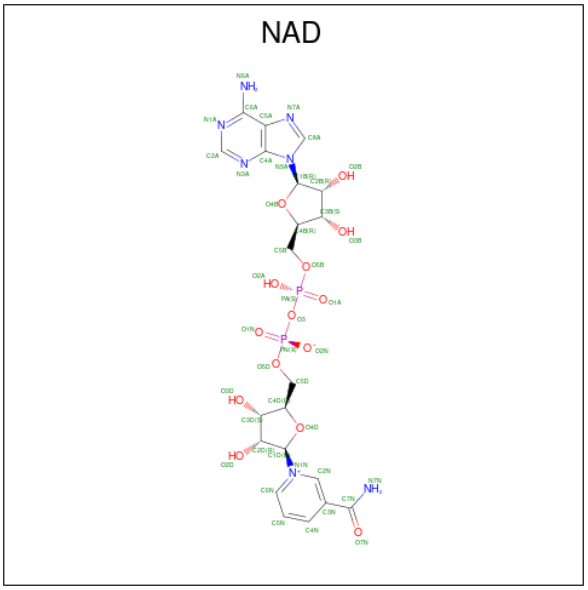
# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2902 atoms, of which 1461 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called tRNA 2'-phosphotransferase.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 178 | 2832 | 896 | 1435 | 248 | 247 | 6 | 0 |

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).




| Mol | Chain | Residues | Atoms | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P |
| 2 | A | 1 | 70 | 21 | 26 | 7 | 14 | 2 |

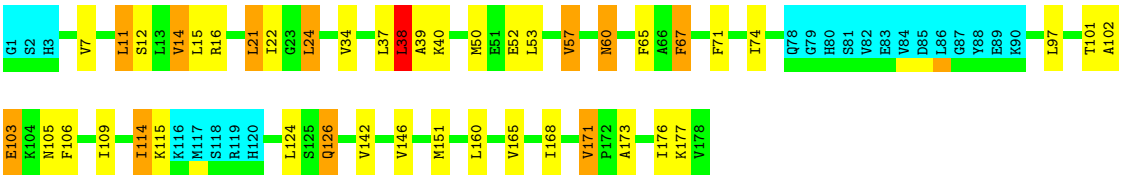
# 4 Residue-property plots

## 4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: tRNA 2'-phosphotransferase

Chain A:



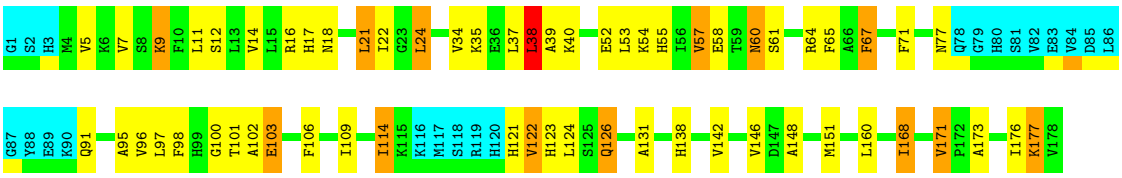

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: tRNA 2'-phosphotransferase

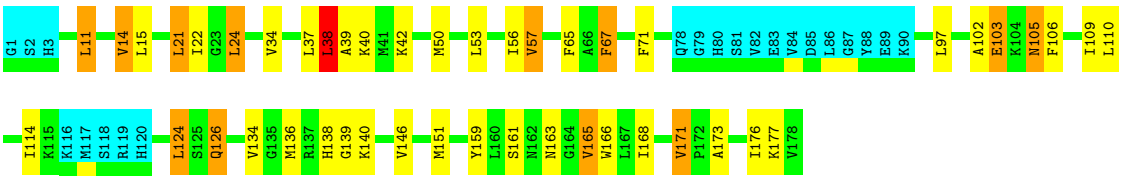
Chain A:




### 4.2.2 Score per residue for model 2

• Molecule 1: tRNA 2'-phosphotransferase

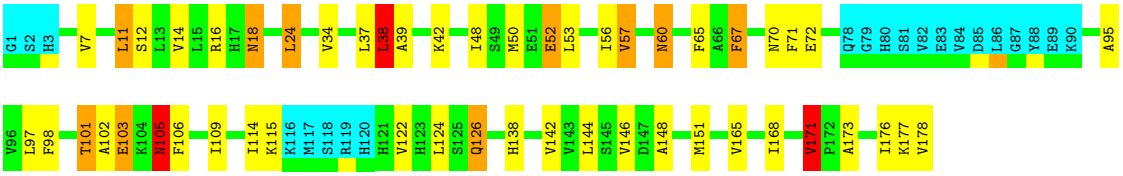
Chain A:



### 4.2.3 Score per residue for model 3

• Molecule 1: tRNA 2'-phosphotransferase

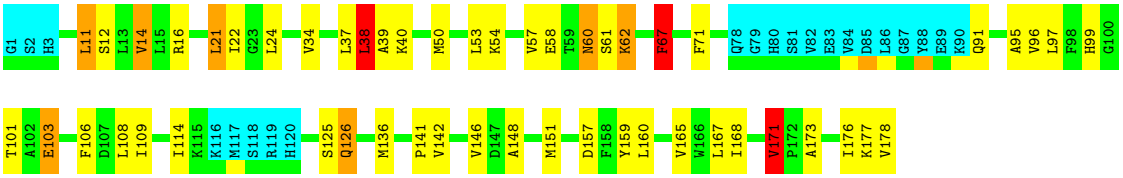
Chain A:



### 4.2.4 Score per residue for model 4

• Molecule 1: tRNA 2'-phosphotransferase

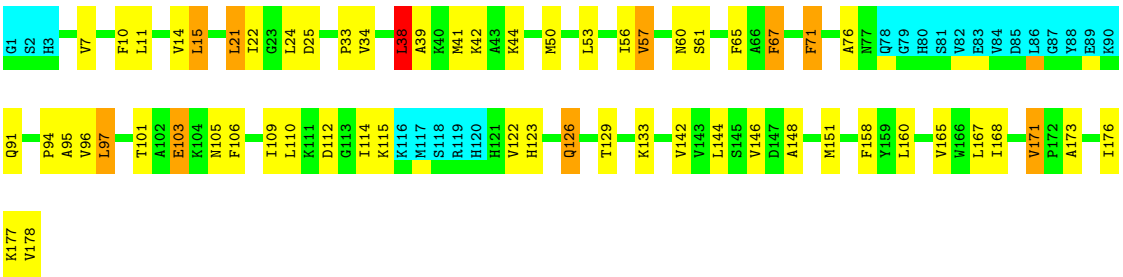
Chain A:



### 4.2.5 Score per residue for model 5

• Molecule 1: tRNA 2'-phosphotransferase

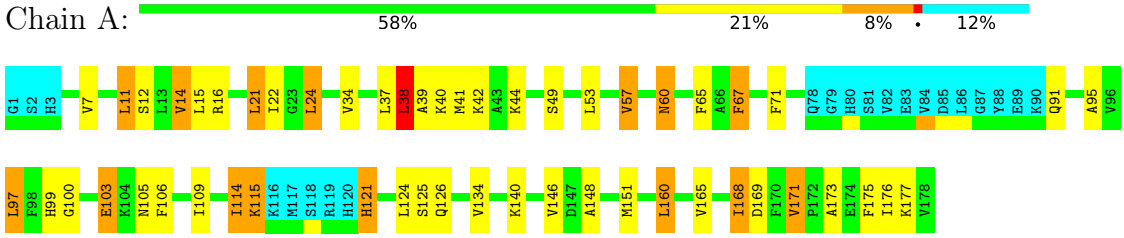
Chain A:



### 4.2.6 Score per residue for model 6

• Molecule 1: tRNA 2'-phosphotransferase

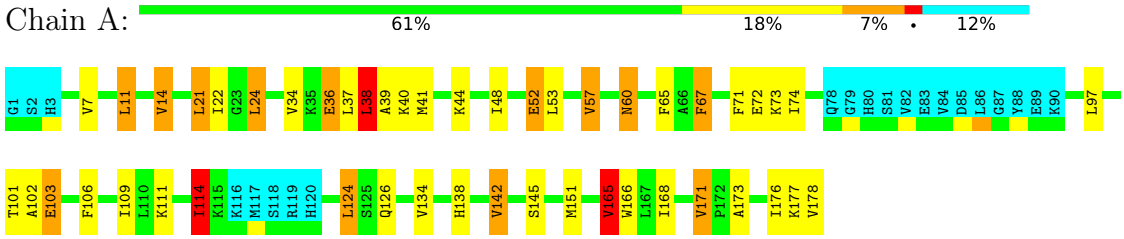
Chain A:




### 4.2.7 Score per residue for model 7

• Molecule 1: tRNA 2'-phosphotransferase

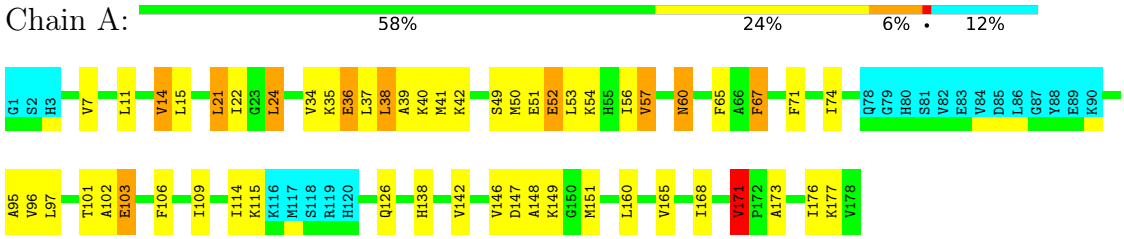
Chain A:




### 4.2.8 Score per residue for model 8

• Molecule 1: tRNA 2'-phosphotransferase

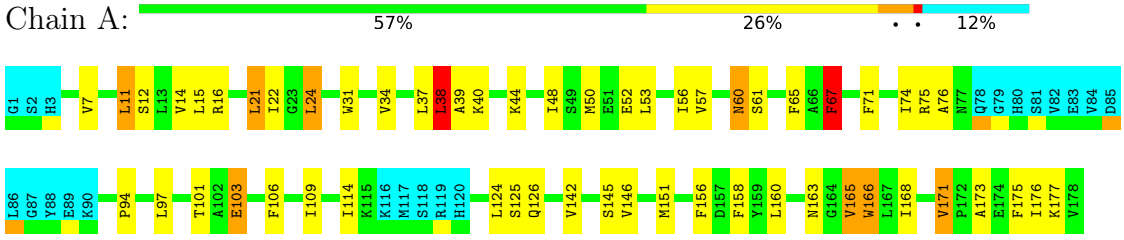
Chain A:




### 4.2.9 Score per residue for model 9

• Molecule 1: tRNA 2'-phosphotransferase

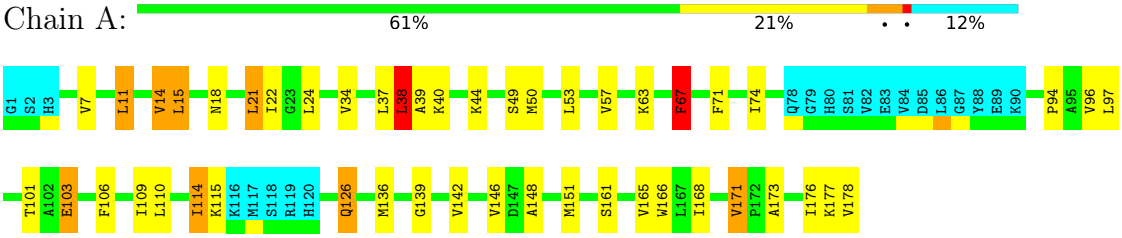
Chain A:



### 4.2.10 Score per residue for model 10

• Molecule 1: tRNA 2'-phosphotransferase

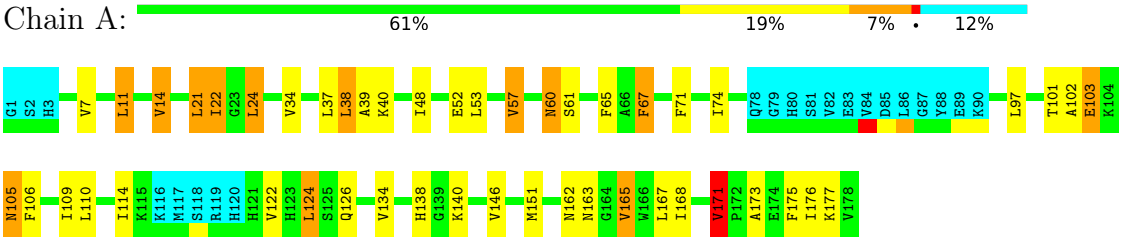
Chain A:




### 4.2.11 Score per residue for model 11

• Molecule 1: tRNA 2'-phosphotransferase

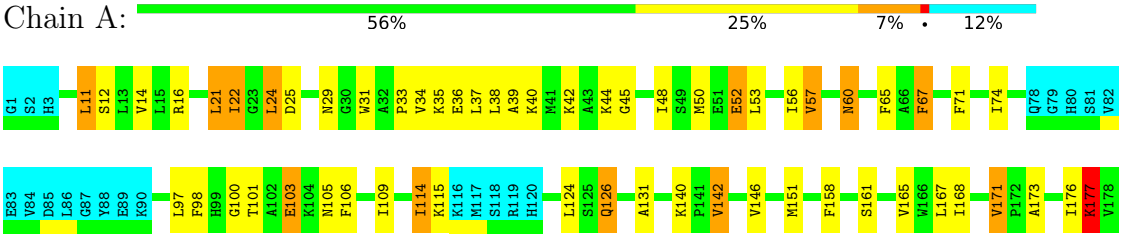
Chain A:




### 4.2.12 Score per residue for model 12

• Molecule 1: tRNA 2'-phosphotransferase

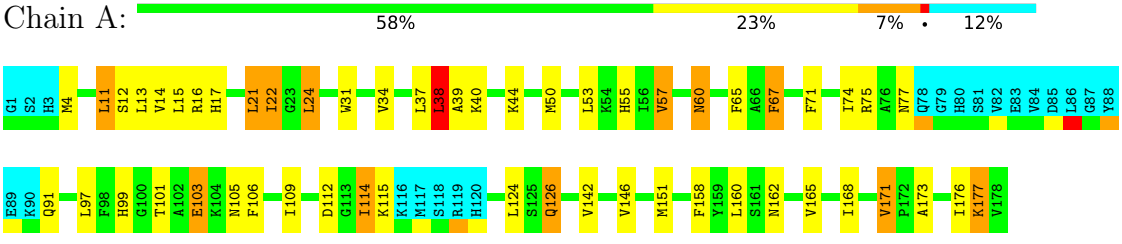
Chain A:




### 4.2.13 Score per residue for model 13

• Molecule 1: tRNA 2'-phosphotransferase

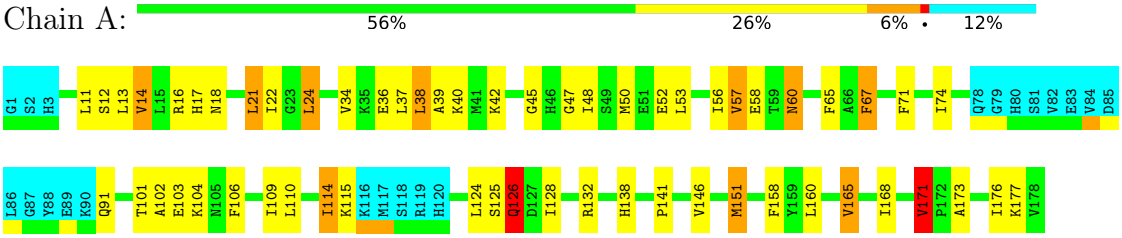
Chain A:



### 4.2.14 Score per residue for model 14

• Molecule 1: tRNA 2'-phosphotransferase

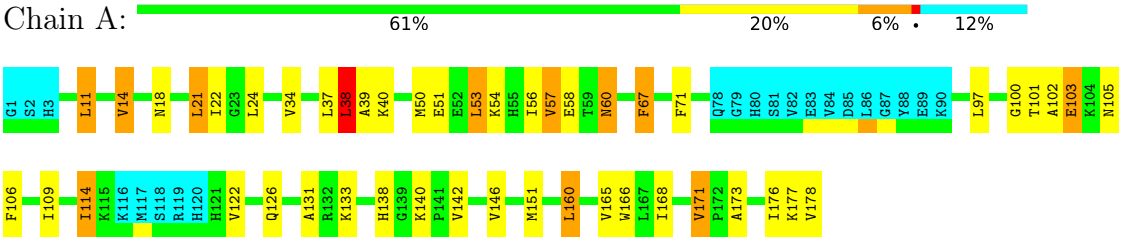
Chain A:




### 4.2.15 Score per residue for model 15

• Molecule 1: tRNA 2'-phosphotransferase

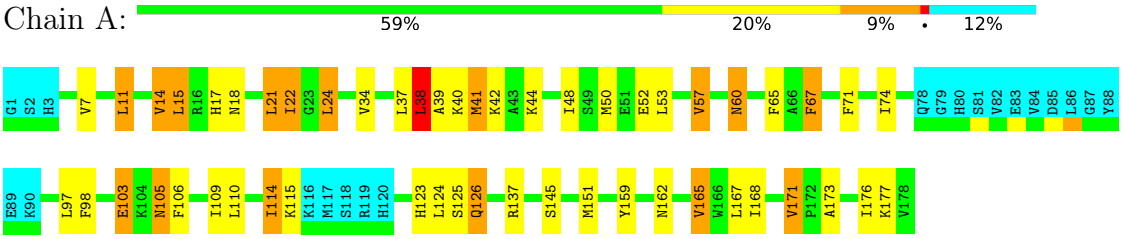
Chain A:




### 4.2.16 Score per residue for model 16

• Molecule 1: tRNA 2'-phosphotransferase

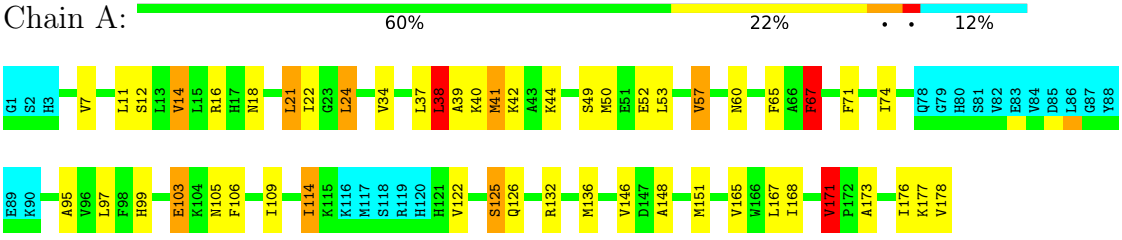
Chain A:




### 4.2.17 Score per residue for model 17

• Molecule 1: tRNA 2'-phosphotransferase

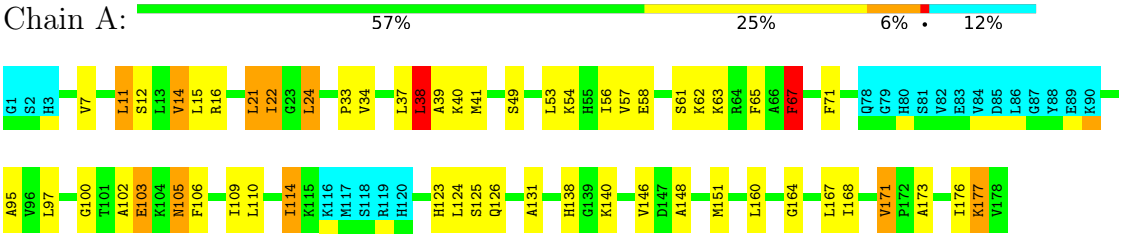
Chain A:



### 4.2.18 Score per residue for model 18

• Molecule 1: tRNA 2'-phosphotransferase

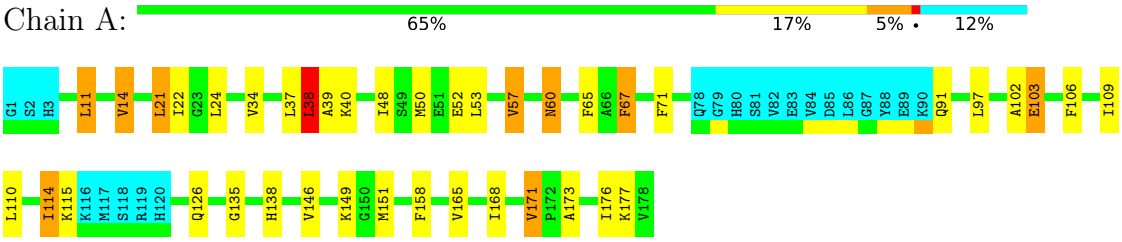
Chain A:




### 4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: tRNA 2'-phosphotransferase

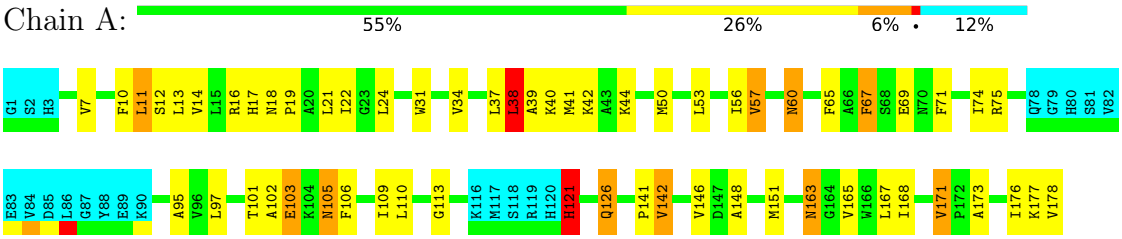
Chain A:




### 4.2.20 Score per residue for model 20

• Molecule 1: tRNA 2'-phosphotransferase

Chain A:



# 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

| Software name | Classification | Version |
|---|---|---|
| ARIA | structure calculation | 2.3.2 |
| X-PLOR NIH | refinement | 2.52 |

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 | 1986 |
| Number of shifts mapped to atoms | 1986 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 81% |

# 6 Model quality

## 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.31±0.03 | 6±2/1258 ( 0.5± 0.1%) | 1.14±0.02 | 3±1/1692 ( 0.2± 0.1%) |
| All | All | 1.31 | 116/25160 ( 0.5%) | 1.14 | 67/33840 ( 0.2%) |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 21 | LEU | N-CA | -8.30 | 1.36 | 1.46 | 11 | 17 |
| 1 | A | 177 | LYS | CA-C | -7.61 | 1.43 | 1.52 | 12 | 12 |
| 1 | A | 177 | LYS | N-CA | -7.59 | 1.37 | 1.46 | 8 | 18 |
| 1 | A | 165 | VAL | CA-C | -7.30 | 1.45 | 1.53 | 9 | 4 |
| 1 | A | 38 | LEU | N-CA | -6.76 | 1.37 | 1.46 | 7 | 18 |
| 1 | A | 24 | LEU | N-CA | -6.57 | 1.37 | 1.45 | 1 | 15 |
| 1 | A | 177 | LYS | C-N | -6.43 | 1.24 | 1.33 | 12 | 15 |
| 1 | A | 114 | ILE | C-N | -6.09 | 1.27 | 1.33 | 7 | 1 |
| 1 | A | 168 | ILE | C-O | 5.85 | 1.29 | 1.24 | 6 | 2 |
| 1 | A | 21 | LEU | CA-C | -5.81 | 1.45 | 1.52 | 1 | 1 |
| 1 | A | 111 | LYS | N-CA | -5.75 | 1.39 | 1.46 | 7 | 1 |
| 1 | A | 17 | HIS | C-N | -5.69 | 1.29 | 1.33 | 1 | 1 |
| 1 | A | 165 | VAL | C-N | -5.67 | 1.25 | 1.33 | 2 | 3 |
| 1 | A | 76 | ALA | N-CA | -5.52 | 1.39 | 1.46 | 9 | 1 |
| 1 | A | 166 | TRP | N-CA | -5.36 | 1.39 | 1.45 | 9 | 1 |
| 1 | A | 35 | LYS | N-CA | -5.32 | 1.39 | 1.46 | 1 | 1 |
| 1 | A | 104 | LYS | C-O | 5.27 | 1.30 | 1.24 | 14 | 1 |
| 1 | A | 100 | GLY | C-N | -5.18 | 1.28 | 1.33 | 6 | 1 |
| 1 | A | 33 | PRO | N-CA | -5.05 | 1.41 | 1.47 | 18 | 1 |
| 1 | A | 125 | SER | N-CA | -5.04 | 1.39 | 1.46 | 9 | 1 |
| 1 | A | 105 | ASN | N-CA | -5.03 | 1.39 | 1.46 | 17 | 1 |

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

occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 122 | VAL | N-CA-C | 9.09 | 119.73 | 106.55 | 1 | 1 |
| 1 | A | 105 | ASN | CA-CB-CG | 7.98 | 120.58 | 112.60 | 3 | 6 |
| 1 | A | 103 | GLU | N-CA-C | 7.73 | 119.71 | 111.28 | 4 | 19 |
| 1 | A | 121 | HIS | CA-C-N | -7.59 | 113.50 | 122.22 | 1 | 2 |
| 1 | A | 121 | HIS | C-N-CA | -7.59 | 113.50 | 122.22 | 1 | 2 |
| 1 | A | 171 | VAL | N-CA-C | 6.65 | 114.73 | 108.15 | 11 | 6 |
| 1 | A | 125 | SER | CA-C-N | 6.57 | 129.41 | 120.54 | 17 | 2 |
| 1 | A | 125 | SER | C-N-CA | 6.57 | 129.41 | 120.54 | 17 | 2 |
| 1 | A | 14 | VAL | N-CA-C | 6.18 | 116.23 | 110.42 | 6 | 13 |
| 1 | A | 163 | ASN | CA-CB-CG | 5.95 | 118.55 | 112.60 | 20 | 1 |
| 1 | A | 121 | HIS | CA-CB-CG | 5.85 | 119.65 | 113.80 | 20 | 1 |
| 1 | A | 67 | PHE | CA-CB-CG | 5.72 | 119.52 | 113.80 | 18 | 5 |
| 1 | A | 22 | ILE | N-CA-C | -5.47 | 106.49 | 113.22 | 18 | 5 |
| 1 | A | 71 | PHE | N-CA-C | -5.28 | 106.14 | 112.58 | 5 | 1 |
| 1 | A | 105 | ASN | N-CA-C | -5.23 | 106.16 | 112.54 | 11 | 1 |

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 1231 | 1275 | 1268 | 43±5 |
| 2 | A | 44 | 26 | 26 | 1±1 |
| All | All | 25500 | 26020 | 25880 | 865 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:14:VAL:HG23 | 1:A:21:LEU:HD21 | 0.80 | 1.52 | 5 | 17 |
| 1:A:38:LEU:HG | 1:A:39:ALA:N | 0.76 | 1.95 | 16 | 20 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:168:ILE:HD13 | 1:A:171:VAL:HG13 | 0.76 | 1.58 | 4 | 20 |
| 1:A:165:VAL:HG11 | 2:A:201:NAD:C6N | 0.70 | 2.17 | 7 | 11 |
| 1:A:106:PHE:HA | 1:A:109:ILE:HG22 | 0.68 | 1.66 | 4 | 20 |
| 1:A:34:VAL:HG13 | 1:A:53:LEU:HD13 | 0.68 | 1.66 | 5 | 4 |
| 1:A:67:PHE:CE2 | 1:A:71:PHE:HB3 | 0.67 | 2.23 | 4 | 20 |
| 1:A:146:VAL:HG11 | 1:A:171:VAL:HG11 | 0.67 | 1.67 | 3 | 15 |
| 1:A:11:LEU:HA | 1:A:14:VAL:HG12 | 0.65 | 1.66 | 12 | 17 |
| 1:A:126:GLN:HE21 | 1:A:126:GLN:N | 0.65 | 1.90 | 10 | 1 |
| 1:A:57:VAL:HG11 | 1:A:67:PHE:CG | 0.65 | 2.28 | 16 | 20 |
| 1:A:37:LEU:HG | 1:A:53:LEU:HD11 | 0.63 | 1.68 | 6 | 19 |
| 1:A:151:MET:HE3 | 1:A:171:VAL:HG12 | 0.63 | 1.68 | 17 | 13 |
| 1:A:67:PHE:CD2 | 1:A:71:PHE:HB3 | 0.62 | 2.29 | 13 | 7 |
| 1:A:12:SER:O | 1:A:16:ARG:HB3 | 0.62 | 1.94 | 12 | 10 |
| 1:A:14:VAL:HG23 | 1:A:21:LEU:CD2 | 0.62 | 2.24 | 5 | 17 |
| 1:A:37:LEU:O | 1:A:41:MET:HB3 | 0.62 | 1.94 | 16 | 2 |
| 1:A:34:VAL:O | 1:A:38:LEU:HD23 | 0.61 | 1.94 | 18 | 20 |
| 1:A:10:PHE:HZ | 1:A:22:ILE:HG21 | 0.61 | 1.56 | 5 | 1 |
| 1:A:21:LEU:HG | 1:A:22:ILE:HG23 | 0.61 | 1.72 | 5 | 3 |
| 1:A:163:ASN:HB2 | 1:A:165:VAL:HG13 | 0.61 | 1.72 | 2 | 1 |
| 1:A:126:GLN:NE2 | 1:A:126:GLN:H | 0.60 | 1.93 | 1 | 4 |
| 1:A:21:LEU:O | 1:A:44:LYS:HE3 | 0.60 | 1.95 | 16 | 9 |
| 1:A:101:THR:HG23 | 1:A:142:VAL:HG13 | 0.60 | 1.73 | 12 | 12 |
| 1:A:126:GLN:HE21 | 1:A:165:VAL:HG12 | 0.60 | 1.56 | 2 | 5 |
| 1:A:57:VAL:HG11 | 1:A:67:PHE:CD1 | 0.59 | 2.32 | 18 | 20 |
| 1:A:126:GLN:H | 1:A:126:GLN:CD | 0.59 | 2.06 | 11 | 5 |
| 1:A:39:ALA:O | 1:A:42:LYS:HB3 | 0.58 | 1.98 | 12 | 9 |
| 1:A:14:VAL:HA | 1:A:21:LEU:HD21 | 0.58 | 1.73 | 12 | 5 |
| 1:A:22:ILE:O | 1:A:40:LYS:HB3 | 0.58 | 1.98 | 12 | 17 |
| 1:A:102:ALA:HA | 1:A:140:LYS:O | 0.58 | 1.99 | 15 | 2 |
| 1:A:10:PHE:CZ | 1:A:22:ILE:HG21 | 0.57 | 2.34 | 5 | 1 |
| 1:A:115:LYS:O | 1:A:121:HIS:HA | 0.57 | 1.99 | 6 | 1 |
| 1:A:7:VAL:HG13 | 1:A:41:MET:SD | 0.56 | 2.39 | 6 | 4 |
| 1:A:151:MET:HE2 | 1:A:171:VAL:HG12 | 0.56 | 1.75 | 6 | 2 |
| 1:A:21:LEU:HG | 1:A:22:ILE:N | 0.56 | 2.16 | 18 | 17 |
| 1:A:173:ALA:HA | 1:A:176:ILE:HD12 | 0.56 | 1.78 | 14 | 20 |
| 1:A:103:GLU:O | 1:A:106:PHE:HB3 | 0.56 | 2.01 | 1 | 19 |
| 1:A:53:LEU:HA | 1:A:56:ILE:HD13 | 0.56 | 1.78 | 2 | 10 |
| 1:A:146:VAL:HB | 1:A:151:MET:SD | 0.55 | 2.42 | 11 | 1 |
| 1:A:38:LEU:HD13 | 1:A:50:MET:N | 0.55 | 2.16 | 16 | 15 |
| 1:A:106:PHE:CZ | 1:A:110:LEU:HD22 | 0.55 | 2.36 | 16 | 9 |
| 1:A:168:ILE:HD13 | 1:A:171:VAL:CG1 | 0.55 | 2.32 | 6 | 15 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:103:GLU:CD | 1:A:140:LYS:HD2 | 0.54 | 2.27 | 11 | 1 |
| 1:A:100:GLY:HA3 | 1:A:131:ALA:O | 0.54 | 2.02 | 1 | 3 |
| 1:A:97:LEU:HD12 | 1:A:124:LEU:HB2 | 0.54 | 1.78 | 6 | 1 |
| 1:A:24:LEU:HD22 | 1:A:37:LEU:HD13 | 0.54 | 1.80 | 9 | 19 |
| 1:A:95:ALA:C | 1:A:148:ALA:HB3 | 0.53 | 2.29 | 5 | 1 |
| 1:A:151:MET:SD | 1:A:175:PHE:HB3 | 0.53 | 2.43 | 6 | 3 |
| 1:A:91:GLN:HG2 | 1:A:160:LEU:HD13 | 0.53 | 1.78 | 5 | 1 |
| 1:A:96:VAL:HB | 1:A:148:ALA:HB2 | 0.53 | 1.79 | 1 | 3 |
| 1:A:126:GLN:HA | 1:A:166:TRP:CE3 | 0.53 | 2.39 | 15 | 2 |
| 1:A:146:VAL:HG11 | 1:A:171:VAL:CG1 | 0.52 | 2.34 | 3 | 12 |
| 1:A:10:PHE:CD2 | 1:A:11:LEU:HD12 | 0.52 | 2.39 | 5 | 1 |
| 1:A:37:LEU:O | 1:A:41:MET:HG2 | 0.52 | 2.04 | 8 | 4 |
| 1:A:34:VAL:HG21 | 1:A:67:PHE:CE1 | 0.52 | 2.40 | 18 | 17 |
| 1:A:101:THR:O | 1:A:141:PRO:HA | 0.52 | 2.04 | 20 | 2 |
| 1:A:136:MET:HA | 1:A:139:GLY:O | 0.52 | 2.05 | 2 | 2 |
| 1:A:109:ILE:HD11 | 1:A:114:ILE:HD12 | 0.52 | 1.80 | 6 | 1 |
| 1:A:15:LEU:HD21 | 1:A:76:ALA:HB2 | 0.51 | 1.81 | 5 | 1 |
| 1:A:57:VAL:HG11 | 1:A:67:PHE:CD2 | 0.51 | 2.41 | 15 | 12 |
| 1:A:62:LYS:HA | 1:A:157:ASP:OD2 | 0.51 | 2.05 | 4 | 1 |
| 1:A:14:VAL:HB | 1:A:21:LEU:HD12 | 0.51 | 1.83 | 20 | 2 |
| 1:A:7:VAL:O | 1:A:11:LEU:HB2 | 0.51 | 2.04 | 20 | 4 |
| 1:A:50:MET:CE | 1:A:71:PHE:HB2 | 0.51 | 2.35 | 16 | 6 |
| 1:A:12:SER:O | 1:A:16:ARG:HG2 | 0.51 | 2.04 | 20 | 1 |
| 1:A:57:VAL:HG23 | 1:A:65:PHE:HB3 | 0.51 | 1.82 | 3 | 16 |
| 1:A:4:MET:HE3 | 1:A:55:HIS:HB3 | 0.51 | 1.82 | 13 | 1 |
| 1:A:54:LYS:O | 1:A:58:GLU:HG3 | 0.51 | 2.05 | 15 | 1 |
| 1:A:97:LEU:HD12 | 1:A:124:LEU:HD21 | 0.51 | 1.80 | 2 | 1 |
| 1:A:91:GLN:NE2 | 1:A:160:LEU:HB2 | 0.50 | 2.21 | 13 | 4 |
| 1:A:52:GLU:O | 1:A:55:HIS:HB3 | 0.50 | 2.06 | 1 | 1 |
| 1:A:11:LEU:O | 1:A:15:LEU:HD22 | 0.50 | 2.07 | 5 | 1 |
| 1:A:18:ASN:O | 1:A:21:LEU:HD23 | 0.50 | 2.06 | 17 | 5 |
| 1:A:114:ILE:HG12 | 1:A:176:ILE:HD11 | 0.50 | 1.84 | 17 | 5 |
| 1:A:14:VAL:HA | 1:A:18:ASN:O | 0.50 | 2.07 | 3 | 1 |
| 1:A:102:ALA:HB3 | 1:A:105:ASN:HB3 | 0.50 | 1.84 | 3 | 2 |
| 1:A:64:ARG:HA | 1:A:77:ASN:O | 0.50 | 2.06 | 1 | 1 |
| 1:A:102:ALA:HB2 | 1:A:138:HIS:HB2 | 0.50 | 1.82 | 3 | 2 |
| 1:A:98:PHE:O | 1:A:124:LEU:HB3 | 0.49 | 2.07 | 3 | 3 |
| 1:A:163:ASN:CB | 1:A:165:VAL:HG13 | 0.49 | 2.36 | 9 | 3 |
| 1:A:95:ALA:O | 1:A:148:ALA:HA | 0.49 | 2.07 | 6 | 7 |
| 1:A:176:ILE:C | 1:A:177:LYS:HD3 | 0.49 | 2.32 | 12 | 1 |
| 1:A:54:LYS:O | 1:A:58:GLU:HB2 | 0.49 | 2.07 | 4 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:50:MET:HE1 | 1:A:71:PHE:HB2 | 0.49 | 1.84 | 17 | 3 |
| 1:A:134:VAL:HG11 | 2:A:201:NAD:H51N | 0.49 | 1.83 | 6 | 2 |
| 1:A:168:ILE:HG21 | 1:A:171:VAL:HG13 | 0.49 | 1.85 | 10 | 5 |
| 1:A:126:GLN:OE1 | 1:A:165:VAL:HA | 0.49 | 2.07 | 17 | 1 |
| 1:A:91:GLN:HE21 | 1:A:160:LEU:HB2 | 0.49 | 1.67 | 5 | 1 |
| 1:A:176:ILE:O | 1:A:177:LYS:HD3 | 0.49 | 2.07 | 1 | 3 |
| 1:A:10:PHE:HD2 | 1:A:11:LEU:HD12 | 0.48 | 1.67 | 5 | 1 |
| 1:A:10:PHE:CZ | 1:A:21:LEU:HD13 | 0.48 | 2.42 | 20 | 1 |
| 1:A:109:ILE:CG1 | 1:A:114:ILE:HD13 | 0.48 | 2.38 | 19 | 8 |
| 1:A:136:MET:SD | 1:A:141:PRO:HG3 | 0.48 | 2.49 | 4 | 1 |
| 1:A:57:VAL:O | 1:A:60:ASN:HB3 | 0.48 | 2.08 | 8 | 15 |
| 1:A:102:ALA:CB | 1:A:138:HIS:HB2 | 0.48 | 2.39 | 7 | 8 |
| 1:A:124:LEU:HD13 | 1:A:168:ILE:HG22 | 0.48 | 1.86 | 18 | 2 |
| 1:A:25:ASP:O | 1:A:33:PRO:HD3 | 0.48 | 2.09 | 5 | 2 |
| 1:A:168:ILE:CD1 | 1:A:171:VAL:HG13 | 0.48 | 2.37 | 5 | 1 |
| 1:A:124:LEU:O | 1:A:165:VAL:HB | 0.48 | 2.08 | 13 | 1 |
| 1:A:36:GLU:O | 1:A:40:LYS:HB2 | 0.48 | 2.09 | 8 | 3 |
| 1:A:114:ILE:O | 1:A:171:VAL:HG23 | 0.48 | 2.09 | 16 | 1 |
| 1:A:124:LEU:CD2 | 1:A:166:TRP:HB2 | 0.48 | 2.38 | 2 | 2 |
| 1:A:158:PHE:CE1 | 1:A:168:ILE:HD12 | 0.48 | 2.44 | 14 | 1 |
| 1:A:151:MET:HE3 | 1:A:151:MET:HA | 0.48 | 1.86 | 2 | 2 |
| 1:A:99:HIS:HA | 1:A:125:SER:OG | 0.48 | 2.08 | 17 | 2 |
| 1:A:35:LYS:HA | 1:A:38:LEU:CD2 | 0.48 | 2.39 | 8 | 1 |
| 1:A:160:LEU:HD11 | 1:A:164:GLY:HA2 | 0.48 | 1.85 | 18 | 1 |
| 1:A:114:ILE:C | 1:A:122:VAL:HG11 | 0.47 | 2.34 | 1 | 1 |
| 1:A:147:ASP:OD2 | 1:A:149:LYS:HG2 | 0.47 | 2.09 | 8 | 1 |
| 1:A:134:VAL:HG11 | 2:A:201:NAD:H4D | 0.47 | 1.86 | 7 | 1 |
| 1:A:11:LEU:O | 1:A:15:LEU:HD23 | 0.47 | 2.09 | 13 | 1 |
| 1:A:123:HIS:CE1 | 1:A:167:LEU:HD12 | 0.47 | 2.44 | 18 | 1 |
| 1:A:57:VAL:HG21 | 1:A:67:PHE:CD1 | 0.47 | 2.44 | 17 | 4 |
| 1:A:126:GLN:HA | 1:A:166:TRP:CD2 | 0.47 | 2.44 | 15 | 1 |
| 1:A:122:VAL:O | 1:A:167:LEU:HG | 0.47 | 2.10 | 11 | 2 |
| 1:A:37:LEU:CD2 | 1:A:74:ILE:HG21 | 0.47 | 2.40 | 20 | 11 |
| 1:A:112:ASP:OD2 | 1:A:115:LYS:HD3 | 0.47 | 2.10 | 13 | 1 |
| 1:A:22:ILE:O | 1:A:40:LYS:HE3 | 0.47 | 2.10 | 1 | 2 |
| 1:A:62:LYS:N | 1:A:62:LYS:HE2 | 0.47 | 2.24 | 4 | 1 |
| 1:A:103:GLU:HA | 1:A:106:PHE:HB3 | 0.47 | 1.87 | 13 | 4 |
| 1:A:114:ILE:HB | 1:A:171:VAL:HG23 | 0.47 | 1.86 | 15 | 4 |
| 1:A:42:LYS:HG3 | 1:A:47:GLY:HA2 | 0.47 | 1.86 | 14 | 1 |
| 1:A:13:LEU:O | 1:A:17:HIS:HB2 | 0.46 | 2.10 | 20 | 2 |
| 1:A:159:TYR:CE1 | 1:A:167:LEU:HD22 | 0.46 | 2.44 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:165:VAL:HG23 | 1:A:167:LEU:CD1 | 0.46 | 2.41 | 20 | 1 |
| 1:A:103:GLU:HA | 1:A:106:PHE:CB | 0.46 | 2.40 | 9 | 8 |
| 1:A:18:ASN:ND2 | 1:A:21:LEU:HD21 | 0.46 | 2.26 | 20 | 1 |
| 1:A:94:PRO:HG3 | 1:A:166:TRP:CD1 | 0.46 | 2.46 | 10 | 1 |
| 1:A:11:LEU:HD21 | 1:A:53:LEU:HD21 | 0.46 | 1.88 | 14 | 1 |
| 1:A:137:ARG:NE | 1:A:137:ARG:HA | 0.46 | 2.26 | 16 | 1 |
| 1:A:48:ILE:HB | 1:A:52:GLU:CB | 0.45 | 2.41 | 16 | 2 |
| 1:A:134:VAL:HG11 | 2:A:201:NAD:H3D | 0.45 | 1.88 | 2 | 1 |
| 1:A:54:LYS:O | 1:A:57:VAL:HG12 | 0.45 | 2.11 | 15 | 1 |
| 1:A:13:LEU:HA | 1:A:17:HIS:CD2 | 0.45 | 2.46 | 14 | 1 |
| 1:A:148:ALA:HA | 1:A:151:MET:HB3 | 0.45 | 1.87 | 5 | 1 |
| 1:A:112:ASP:CG | 1:A:115:LYS:HD3 | 0.45 | 2.37 | 13 | 1 |
| 1:A:49:SER:HB3 | 1:A:52:GLU:OE2 | 0.45 | 2.12 | 17 | 1 |
| 1:A:106:PHE:HB2 | 1:A:142:VAL:HG11 | 0.45 | 1.89 | 4 | 2 |
| 1:A:161:SER:HB2 | 1:A:165:VAL:CG2 | 0.45 | 2.41 | 2 | 1 |
| 1:A:105:ASN:ND2 | 2:A:201:NAD:H1B | 0.45 | 2.27 | 5 | 3 |
| 1:A:129:THR:O | 1:A:133:LYS:HB2 | 0.45 | 2.11 | 5 | 1 |
| 1:A:38:LEU:HD13 | 1:A:49:SER:C | 0.45 | 2.37 | 18 | 4 |
| 1:A:108:LEU:HB2 | 2:A:201:NAD:H2A | 0.45 | 1.89 | 4 | 1 |
| 1:A:31:TRP:CE3 | 1:A:75:ARG:HB2 | 0.44 | 2.48 | 20 | 2 |
| 1:A:21:LEU:HG | 1:A:22:ILE:H | 0.44 | 1.72 | 14 | 5 |
| 1:A:17:HIS:CE1 | 1:A:162:ASN:HB2 | 0.44 | 2.47 | 16 | 1 |
| 1:A:97:LEU:O | 1:A:145:SER:HA | 0.44 | 2.11 | 16 | 3 |
| 1:A:15:LEU:H | 1:A:15:LEU:HD23 | 0.44 | 1.73 | 16 | 5 |
| 1:A:10:PHE:CD2 | 1:A:10:PHE:C | 0.44 | 2.95 | 5 | 1 |
| 1:A:165:VAL:HG21 | 2:A:201:NAD:C5N | 0.44 | 2.42 | 19 | 1 |
| 1:A:48:ILE:HB | 1:A:52:GLU:HB2 | 0.43 | 1.90 | 3 | 7 |
| 1:A:94:PRO:HD2 | 1:A:158:PHE:CE2 | 0.43 | 2.48 | 9 | 1 |
| 2:A:201:NAD:H3B | 2:A:201:NAD:O3 | 0.43 | 2.12 | 17 | 1 |
| 1:A:144:LEU:HD23 | 1:A:178:VAL:HA | 0.43 | 1.90 | 5 | 2 |
| 1:A:151:MET:CE | 1:A:171:VAL:HG12 | 0.43 | 2.43 | 15 | 5 |
| 1:A:103:GLU:OE2 | 1:A:140:LYS:HG2 | 0.43 | 2.13 | 2 | 1 |
| 1:A:115:LYS:O | 1:A:122:VAL:HB | 0.43 | 2.13 | 5 | 1 |
| 1:A:98:PHE:O | 1:A:125:SER:HB2 | 0.43 | 2.13 | 16 | 1 |
| 1:A:29:ASN:HD22 | 1:A:31:TRP:NE1 | 0.43 | 2.12 | 12 | 1 |
| 1:A:173:ALA:O | 1:A:176:ILE:HB | 0.43 | 2.13 | 20 | 2 |
| 1:A:114:ILE:HG22 | 1:A:122:VAL:HG21 | 0.43 | 1.90 | 5 | 2 |
| 1:A:91:GLN:NE2 | 1:A:160:LEU:HD22 | 0.43 | 2.28 | 5 | 1 |
| 1:A:49:SER:HB2 | 1:A:52:GLU:OE1 | 0.43 | 2.13 | 8 | 1 |
| 1:A:160:LEU:HA | 1:A:165:VAL:O | 0.43 | 2.14 | 8 | 2 |
| 1:A:91:GLN:HB2 | 1:A:160:LEU:HD13 | 0.43 | 1.91 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:7:VAL:HG13 | 1:A:41:MET:CE | 0.43 | 2.43 | 5 | 1 |
| 1:A:126:GLN:NE2 | 1:A:165:VAL:HG12 | 0.43 | 2.25 | 2 | 2 |
| 1:A:70:ASN:HD22 | 1:A:72:GLU:HB2 | 0.43 | 1.74 | 3 | 1 |
| 1:A:38:LEU:O | 1:A:42:LYS:HB2 | 0.43 | 2.14 | 17 | 2 |
| 1:A:53:LEU:O | 1:A:53:LEU:HD23 | 0.42 | 2.14 | 5 | 3 |
| 1:A:31:TRP:CD2 | 1:A:75:ARG:HB2 | 0.42 | 2.50 | 9 | 1 |
| 1:A:69:GLU:H | 1:A:69:GLU:CD | 0.42 | 2.23 | 20 | 1 |
| 1:A:113:GLY:HA2 | 1:A:173:ALA:HB2 | 0.42 | 1.91 | 20 | 1 |
| 1:A:114:ILE:HG12 | 1:A:171:VAL:CG2 | 0.42 | 2.44 | 6 | 1 |
| 1:A:151:MET:HB3 | 1:A:158:PHE:CZ | 0.42 | 2.49 | 12 | 2 |
| 1:A:114:ILE:HB | 1:A:171:VAL:CG2 | 0.42 | 2.44 | 15 | 1 |
| 1:A:11:LEU:HD23 | 1:A:65:PHE:CE1 | 0.42 | 2.50 | 18 | 3 |
| 1:A:105:ASN:O | 1:A:109:ILE:HB | 0.42 | 2.15 | 15 | 1 |
| 1:A:106:PHE:HA | 1:A:109:ILE:CG2 | 0.42 | 2.42 | 6 | 3 |
| 1:A:21:LEU:HD23 | 1:A:21:LEU:H | 0.42 | 1.74 | 7 | 1 |
| 1:A:159:TYR:CE2 | 1:A:167:LEU:HD22 | 0.42 | 2.50 | 16 | 1 |
| 1:A:106:PHE:CA | 1:A:109:ILE:HG22 | 0.41 | 2.42 | 7 | 4 |
| 1:A:161:SER:HB2 | 1:A:167:LEU:HD11 | 0.41 | 1.91 | 12 | 1 |
| 1:A:14:VAL:HG22 | 1:A:19:PRO:HA | 0.41 | 1.92 | 20 | 1 |
| 1:A:114:ILE:HD13 | 1:A:176:ILE:HD11 | 0.41 | 1.91 | 6 | 1 |
| 1:A:115:LYS:HG3 | 1:A:169:ASP:O | 0.41 | 2.15 | 6 | 1 |
| 1:A:99:HIS:HB2 | 1:A:124:LEU:HG | 0.41 | 1.92 | 13 | 1 |
| 1:A:5:VAL:O | 1:A:9:LYS:HG2 | 0.41 | 2.14 | 1 | 1 |
| 1:A:95:ALA:HB1 | 1:A:148:ALA:HB1 | 0.41 | 1.92 | 4 | 1 |
| 1:A:100:GLY:N | 1:A:131:ALA:HB1 | 0.41 | 2.30 | 18 | 1 |
| 1:A:146:VAL:HG12 | 1:A:176:ILE:HA | 0.41 | 1.93 | 15 | 1 |
| 1:A:95:ALA:C | 1:A:148:ALA:HA | 0.41 | 2.41 | 17 | 1 |
| 1:A:44:LYS:HD2 | 1:A:44:LYS:C | 0.41 | 2.39 | 20 | 1 |
| 1:A:94:PRO:HD2 | 1:A:158:PHE:CD2 | 0.41 | 2.50 | 5 | 1 |
| 1:A:11:LEU:HD12 | 1:A:41:MET:HE1 | 0.41 | 1.92 | 8 | 1 |
| 1:A:109:ILE:HG12 | 1:A:114:ILE:HD13 | 0.41 | 1.91 | 19 | 1 |
| 1:A:96:VAL:HG23 | 1:A:146:VAL:O | 0.41 | 2.15 | 4 | 1 |
| 1:A:91:GLN:NE2 | 1:A:160:LEU:HD12 | 0.41 | 2.30 | 6 | 1 |
| 1:A:99:HIS:HB2 | 1:A:124:LEU:HA | 0.41 | 1.93 | 6 | 1 |
| 1:A:72:GLU:C | 1:A:73:LYS:HD2 | 0.41 | 2.40 | 7 | 1 |
| 1:A:15:LEU:HD23 | 1:A:15:LEU:H | 0.41 | 1.76 | 10 | 1 |
| 1:A:128:ILE:O | 1:A:132:ARG:HG3 | 0.40 | 2.16 | 14 | 1 |
| 1:A:51:GLU:O | 1:A:54:LYS:HB3 | 0.40 | 2.16 | 15 | 2 |
| 1:A:124:LEU:HD11 | 1:A:168:ILE:HG22 | 0.40 | 1.94 | 11 | 1 |
| 1:A:151:MET:SD | 1:A:168:ILE:HD11 | 0.40 | 2.56 | 16 | 1 |
| 1:A:97:LEU:HG | 1:A:146:VAL:CG2 | 0.40 | 2.46 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:109:ILE:HG13 | 1:A:114:ILE:HG23 | 0.40 | 1.93 | 6 | 1 |
| 1:A:132:ARG:O | 1:A:136:MET:HG3 | 0.40 | 2.16 | 17 | 1 |
| 1:A:14:VAL:CG2 | 1:A:21:LEU:HD21 | 0.40 | 2.34 | 5 | 1 |
| 1:A:102:ALA:HB2 | 1:A:135:GLY:O | 0.40 | 2.17 | 19 | 1 |
| 1:A:112:ASP:O | 1:A:115:LYS:HE3 | 0.40 | 2.15 | 5 | 1 |
| 1:A:102:ALA:HB3 | 1:A:105:ASN:OD1 | 0.40 | 2.17 | 15 | 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 | 156/178 (88%) | 145±3 (93±2%) | 9±2 (6±1%) | 2±1 (1±1%) | 13 | 61 |
| All | All | 3120/3560 (88%) | 2901 (93%) | 181 (6%) | 38 (1%) | 13 | 61 |

All 9 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 | 60 | ASN | 17 |
| 1 | A | 61 | SER | 6 |
| 1 | A | 115 | LYS | 6 |
| 1 | A | 125 | SER | 2 |
| 1 | A | 63 | LYS | 2 |
| 1 | A | 45 | GLY | 2 |
| 1 | A | 126 | GLN | 1 |
| 1 | A | 62 | LYS | 1 |
| 1 | A | 121 | HIS | 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 | 132/150 (88%) | 122±2 (92±1%) | 10±2 (8±1%) | 14 61 |
| All | All | 2640/3000 (88%) | 2436 (92%) | 204 (8%) | 14 61 |

All 40 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 | 67 | PHE | 20 |
| 1 | A | 171 | VAL | 20 |
| 1 | A | 38 | LEU | 17 |
| 1 | A | 114 | ILE | 17 |
| 1 | A | 11 | LEU | 16 |
| 1 | A | 57 | VAL | 16 |
| 1 | A | 97 | LEU | 15 |
| 1 | A | 126 | GLN | 15 |
| 1 | A | 105 | ASN | 6 |
| 1 | A | 124 | LEU | 6 |
| 1 | A | 178 | VAL | 6 |
| 1 | A | 52 | GLU | 4 |
| 1 | A | 15 | LEU | 4 |
| 1 | A | 123 | HIS | 3 |
| 1 | A | 36 | GLU | 3 |
| 1 | A | 142 | VAL | 3 |
| 1 | A | 41 | MET | 3 |
| 1 | A | 18 | ASN | 2 |
| 1 | A | 101 | THR | 2 |
| 1 | A | 115 | LYS | 2 |
| 1 | A | 122 | VAL | 2 |
| 1 | A | 96 | VAL | 2 |
| 1 | A | 140 | LYS | 2 |
| 1 | A | 160 | LEU | 2 |
| 1 | A | 9 | LYS | 1 |
| 1 | A | 159 | TYR | 1 |
| 1 | A | 62 | LYS | 1 |
| 1 | A | 165 | VAL | 1 |
| 1 | A | 156 | PHE | 1 |
| 1 | A | 35 | LYS | 1 |
| 1 | A | 177 | LYS | 1 |
| 1 | A | 158 | PHE | 1 |
| 1 | A | 58 | GLU | 1 |
| 1 | A | 151 | MET | 1 |
| 1 | A | 53 | LEU | 1 |
| 1 | A | 133 | LYS | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 167 | LEU | 1 |
| 1 | A | 149 | LYS | 1 |
| 1 | A | 121 | HIS | 1 |
| 1 | A | 163 | ASN | 1 |

### 6.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | NAD | A | 201 | - | 46,48,48 | 1.86±0.08 | 10±1 (22±2%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | NAD | A | 201 | - | 64,73,73 | 1.76±0.03 | 10±1 (14±0%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | NAD | A | 201 | - | - | 0±0,30,62,62 | 0±0,5,5,5 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 2 | A | 201 | NAD | O4D-C1D | 6.32 | 1.49 | 1.40 | 5 | 20 |
| 2 | A | 201 | NAD | C2N-N1N | 6.03 | 1.41 | 1.35 | 18 | 20 |
| 2 | A | 201 | NAD | C5A-N7A | 5.84 | 1.28 | 1.39 | 19 | 20 |
| 2 | A | 201 | NAD | C4A-N9A | 3.87 | 1.29 | 1.37 | 3 | 20 |
| 2 | A | 201 | NAD | C3N-C7N | 3.77 | 1.56 | 1.50 | 11 | 20 |
| 2 | A | 201 | NAD | C2N-C3N | 3.64 | 1.44 | 1.39 | 12 | 16 |
| 2 | A | 201 | NAD | C8A-N7A | 3.57 | 1.38 | 1.31 | 16 | 20 |
| 2 | A | 201 | NAD | C2D-C3D | 2.86 | 1.45 | 1.53 | 3 | 10 |
| 2 | A | 201 | NAD | C5A-C4A | 2.85 | 1.34 | 1.39 | 17 | 20 |
| 2 | A | 201 | NAD | C2A-N1A | 2.76 | 1.38 | 1.33 | 2 | 9 |
| 2 | A | 201 | NAD | O3B-C3B | 2.41 | 1.48 | 1.43 | 3 | 8 |
| 2 | A | 201 | NAD | C3D-C4D | 2.38 | 1.46 | 1.53 | 2 | 1 |
| 2 | A | 201 | NAD | O4B-C1B | 2.35 | 1.47 | 1.42 | 10 | 7 |
| 2 | A | 201 | NAD | C8A-N9A | 2.32 | 1.41 | 1.37 | 3 | 2 |
| 2 | A | 201 | NAD | C2B-C3B | 2.31 | 1.47 | 1.53 | 7 | 9 |
| 2 | A | 201 | NAD | PA-O3 | 2.04 | 1.61 | 1.59 | 7 | 1 |
| 2 | A | 201 | NAD | C1B-N9A | 2.02 | 1.51 | 1.46 | 1 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 2 | A | 201 | NAD | C5A-C4A-N3A | 6.15 | 118.24 | 126.72 | 7 | 20 |
| 2 | A | 201 | NAD | C6A-C5A-N7A | 5.86 | 120.80 | 132.09 | 19 | 20 |
| 2 | A | 201 | NAD | C6A-C5A-C4A | 5.66 | 124.90 | 117.18 | 19 | 20 |
| 2 | A | 201 | NAD | N3A-C4A-N9A | 4.82 | 135.36 | 127.17 | 7 | 20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 2 | A | 201 | NAD | C4D-O4D-C1D | 4.17 | 106.11 | 109.92 | 11 | 20 |
| 2 | A | 201 | NAD | N9A-C8A-N7A | 4.02 | 108.24 | 113.94 | 3 | 20 |
| 2 | A | 201 | NAD | C6N-N1N-C2N | 3.42 | 118.97 | 121.88 | 15 | 20 |
| 2 | A | 201 | NAD | C4A-C5A-N7A | 3.25 | 114.30 | 110.58 | 19 | 20 |
| 2 | A | 201 | NAD | C2A-N3A-C4A | 2.44 | 117.80 | 111.83 | 16 | 20 |
| 2 | A | 201 | NAD | N3A-C2A-N1A | 2.40 | 124.95 | 128.58 | 20 | 9 |
| 2 | A | 201 | NAD | O4B-C1B-N9A | 2.25 | 112.40 | 108.09 | 3 | 1 |
| 2 | A | 201 | NAD | C2N-N1N-C1D | 2.04 | 123.65 | 119.13 | 2 | 1 |

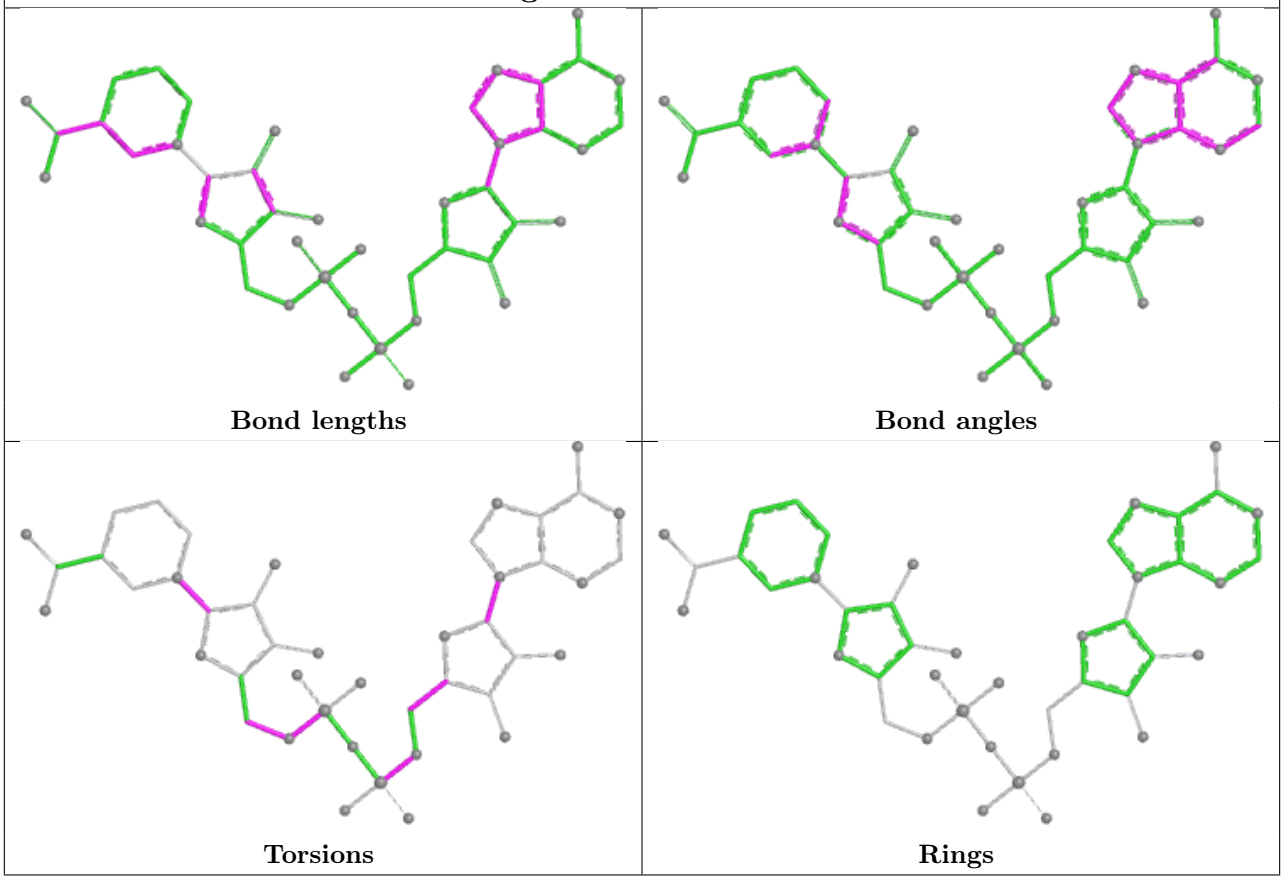
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

**Ligand NAD A 201**




## 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

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 79% 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

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 | 1986 |
| Number of shifts mapped to atoms | 1986 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 1 |

### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 161 | -0.08 ± 0.10 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 137 | 0.10 ± 0.15 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 146 | 0.00 ± 0.13 | None needed (< 0.5 ppm) |
| $^{15}N$ | 159 | 0.41 ± 0.32 | None needed (< 0.5 ppm) |

### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1773 atoms were assigned a chemical shift out of a possible 2192. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 718/785 (91%) | 295/320 (92%) | 279/314 (89%) | 144/151 (95%) |
| Sidechain | 969/1218 (80%) | 652/797 (82%) | 307/379 (81%) | 10/42 (24%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 86/189 (46%) | 45/94 (48%) | 39/79 (49%) | 2/16 (12%) |
| Overall | 1773/2192 (81%) | 992/1211 (82%) | 625/772 (81%) | 156/209 (75%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1950 atoms were assigned a chemical shift out of a possible 2469. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 793/893 (89%) | 327/365 (90%) | 307/356 (86%) | 159/172 (92%) |
| Sidechain | 1057/1354 (78%) | 712/884 (81%) | 334/422 (79%) | 11/48 (23%) |
| Aromatic | 100/222 (45%) | 52/110 (47%) | 46/90 (51%) | 2/22 (9%) |
| Overall | 1950/2469 (79%) | 1091/1359 (80%) | 687/868 (79%) | 172/242 (71%) |

### 7.1.4 Statistically unusual chemical shifts (i)

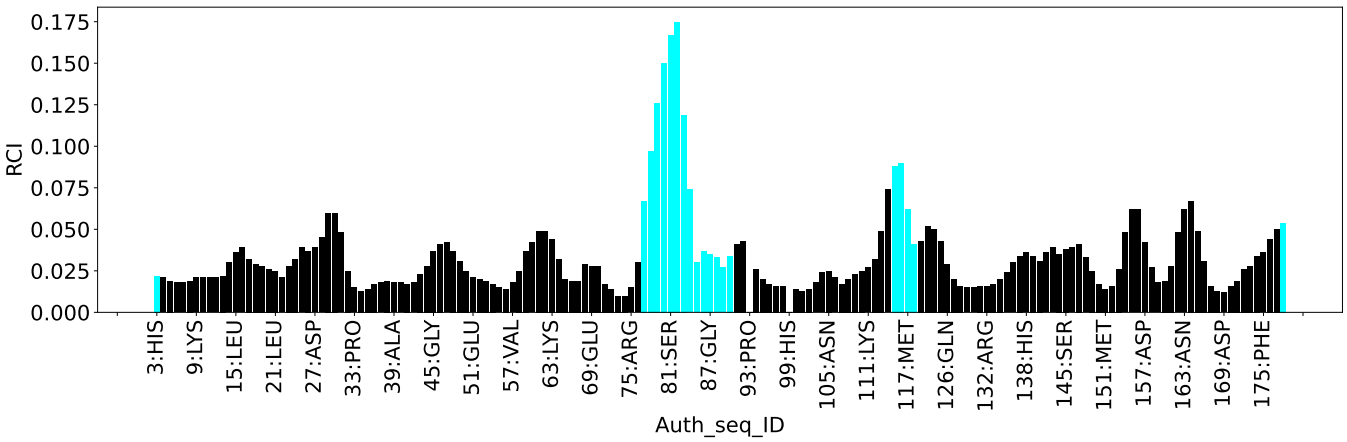
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, *ppm* | Expected range, *ppm* | Z-score |
|---|---|---|---|---|---|---|---|
| 1 | A | 123 | HIS | CD2 | 137.98 | 103.95 – 136.66 | 5.4 |

### 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:


RCI
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
3:HIS
9:LYS
15:LEU
21:LEU
27:ASP
33:PRO
39:ALA
45:GLY
51:GLU
57:VAL
63:LYS
69:GLU
75:ARG
81:SER
87:GLY
93:PRO
99:HIS
105:ASN
111:LYS
117:MET
126:GLN
132:ARG
138:HIS
145:SER
151:MET
157:ASP
163:ASN
169:ASP
175:PHE
Auth_seq_ID

# 8 NMR restraints analysis

## 8.1 Conformationally restricting restraints

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

| Description | Value |
|---|---|
| Total distance restraints | 4573 |
| Intra-residue (\|i-j\|=0) | 1606 |
| Sequential (\|i-j\|=1) | 1068 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 684 |
| Long range (\|i-j\|≥5) | 990 |
| Inter-chain | 99 |
| Hydrogen bond restraints | 126 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 269 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 27.1 |
| Number of long range restraints per residue[1] | 5.7 |

[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

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

### 8.2.1 Average number of distance violations per model

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

| Bins (Å) | Average number of violations per model | Max (Å) |
|---|---|---|
| 0.1-0.2 (Small) | 176.6 | 0.2 |
| 0.2-0.5 (Medium) | 281.5 | 0.5 |
| >0.5 (Large) | 183.4 | 6.05 |

### 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) | 17.0 | 4.91 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

# 9 Distance violation analysis (i)

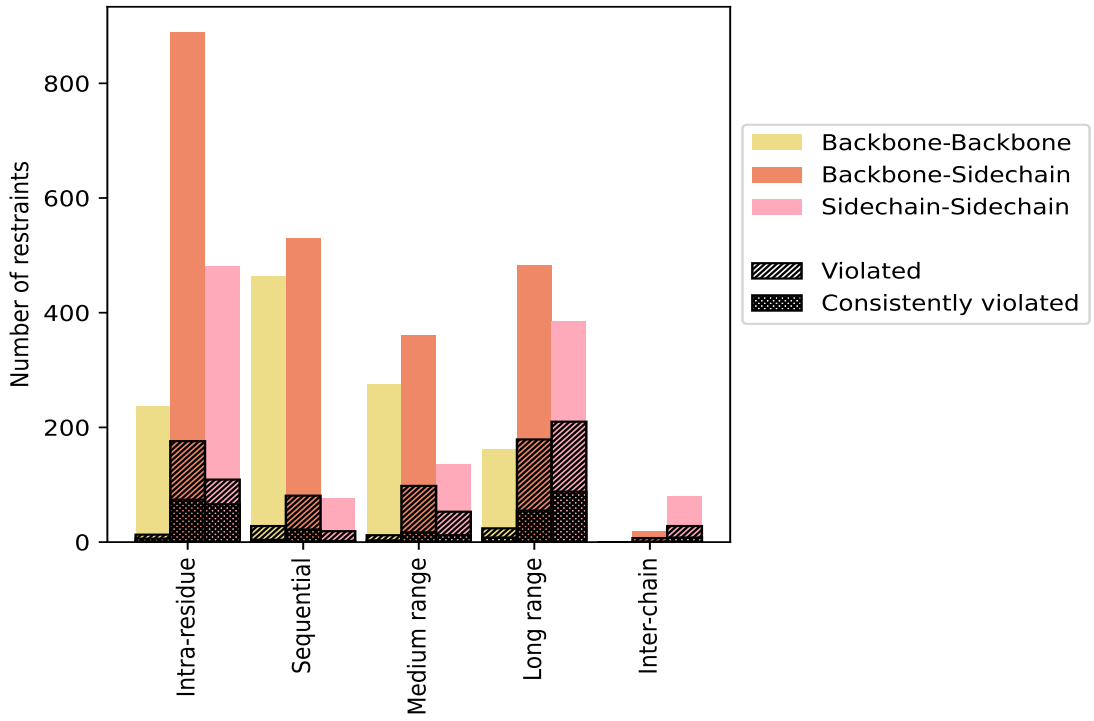
## 9.1 Summary of distance violations (i)

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) | 1606 | 35.1 | 298 | 18.6 | 6.5 | 146 | 9.1 | 3.2 |
| Backbone-Backbone | 237 | 5.2 | 13 | 5.5 | 0.3 | 6 | 2.5 | 0.1 |
| Backbone-Sidechain | 889 | 19.4 | 176 | 19.8 | 3.8 | 74 | 8.3 | 1.6 |
| Sidechain-Sidechain | 480 | 10.5 | 109 | 22.7 | 2.4 | 66 | 13.8 | 1.4 |
| Sequential (\|i-j\|=1) | 1068 | 23.4 | 128 | 12.0 | 2.8 | 28 | 2.6 | 0.6 |
| Backbone-Backbone | 463 | 10.1 | 28 | 6.0 | 0.6 | 4 | 0.9 | 0.1 |
| Backbone-Sidechain | 529 | 11.6 | 81 | 15.3 | 1.8 | 22 | 4.2 | 0.5 |
| Sidechain-Sidechain | 76 | 1.7 | 19 | 25.0 | 0.4 | 2 | 2.6 | 0.0 |
| Medium range (\|i-j\|>1 & \|i-j\|<5) | 684 | 15.0 | 116 | 17.0 | 2.5 | 28 | 4.1 | 0.6 |
| Backbone-Backbone | 275 | 6.0 | 12 | 4.4 | 0.3 | 3 | 1.1 | 0.1 |
| Backbone-Sidechain | 273 | 6.0 | 51 | 18.7 | 1.1 | 13 | 4.8 | 0.3 |
| Sidechain-Sidechain | 136 | 3.0 | 53 | 39.0 | 1.2 | 12 | 8.8 | 0.3 |
| Long range (\|i-j\|≥5) | 990 | 21.6 | 386 | 39.0 | 8.4 | 146 | 14.7 | 3.2 |
| Backbone-Backbone | 162 | 3.5 | 24 | 14.8 | 0.5 | 8 | 4.9 | 0.2 |
| Backbone-Sidechain | 444 | 9.7 | 152 | 34.2 | 3.3 | 50 | 11.3 | 1.1 |
| Sidechain-Sidechain | 384 | 8.4 | 210 | 54.7 | 4.6 | 88 | 22.9 | 1.9 |
| Inter-chain | 99 | 2.2 | 35 | 35.4 | 0.8 | 9 | 9.1 | 0.2 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 19 | 0.4 | 7 | 36.8 | 0.2 | 1 | 5.3 | 0.0 |
| Sidechain-Sidechain | 80 | 1.7 | 28 | 35.0 | 0.6 | 8 | 10.0 | 0.2 |
| Hydrogen bond | 126 | 2.8 | 74 | 58.7 | 1.6 | 9 | 7.1 | 0.2 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 4573 | 100.0 | 1037 | 22.7 | 22.7 | 366 | 8.0 | 8.0 |
| Backbone-Backbone | 1137 | 24.9 | 77 | 6.8 | 1.7 | 21 | 1.8 | 0.5 |
| Backbone-Sidechain | 2280 | 49.9 | 541 | 23.7 | 11.8 | 169 | 7.4 | 3.7 |
| Sidechain-Sidechain | 1156 | 25.3 | 419 | 36.2 | 9.2 | 176 | 15.2 | 3.8 |

[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




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

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 | 199 | 73 | 85 | 253 | 16 | 626 | 0.45 | 3.67 | 0.42 | 0.3 |
| 2 | 218 | 81 | 95 | 270 | 16 | 680 | 0.46 | 6.05 | 0.46 | 0.32 |
| 3 | 207 | 72 | 88 | 250 | 16 | 633 | 0.46 | 3.38 | 0.43 | 0.32 |
| 4 | 213 | 75 | 89 | 259 | 16 | 652 | 0.45 | 3.55 | 0.41 | 0.31 |
| 5 | 212 | 75 | 89 | 272 | 13 | 661 | 0.45 | 3.73 | 0.4 | 0.31 |
| 6 | 208 | 76 | 84 | 257 | 20 | 645 | 0.46 | 4.35 | 0.43 | 0.31 |
| 7 | 214 | 74 | 87 | 255 | 19 | 649 | 0.47 | 3.62 | 0.43 | 0.33 |
| 8 | 206 | 69 | 88 | 253 | 16 | 632 | 0.46 | 3.49 | 0.42 | 0.32 |
| 9 | 216 | 82 | 84 | 270 | 16 | 668 | 0.46 | 5.03 | 0.45 | 0.32 |
| 10 | 218 | 73 | 90 | 248 | 16 | 645 | 0.45 | 4.05 | 0.41 | 0.31 |

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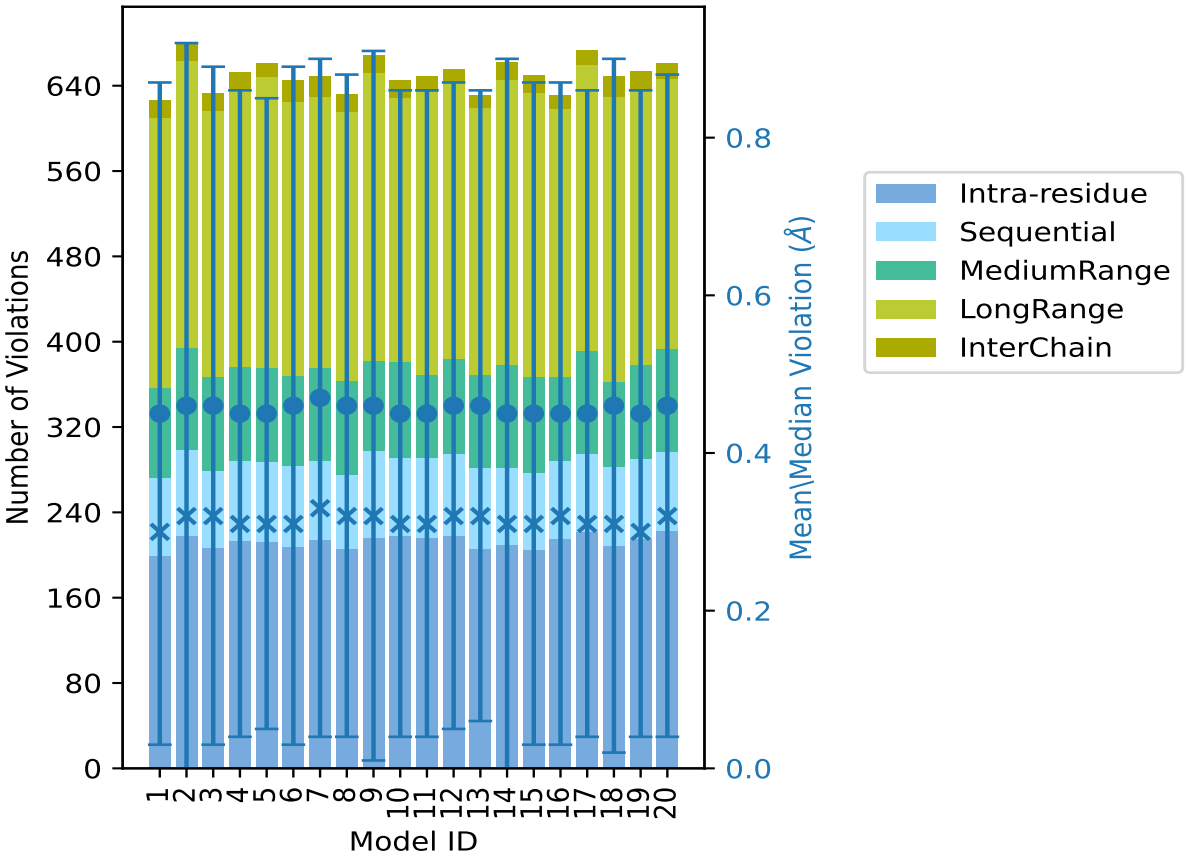
| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 11 | 216 | 75 | 78 | 265 | 15 | 649 | 0.45 | 3.78 | 0.41 | 0.31 |
| 12 | 218 | 77 | 89 | 260 | 12 | 656 | 0.46 | 4.02 | 0.41 | 0.32 |
| 13 | 206 | 76 | 87 | 250 | 12 | 631 | 0.46 | 2.77 | 0.4 | 0.32 |
| 14 | 209 | 73 | 96 | 268 | 16 | 662 | 0.45 | 5.97 | 0.45 | 0.31 |
| 15 | 205 | 72 | 90 | 267 | 16 | 650 | 0.45 | 3.24 | 0.42 | 0.31 |
| 16 | 215 | 74 | 78 | 251 | 13 | 631 | 0.45 | 4.57 | 0.42 | 0.32 |
| 17 | 222 | 73 | 96 | 268 | 14 | 673 | 0.45 | 3.66 | 0.41 | 0.31 |
| 18 | 208 | 75 | 79 | 268 | 19 | 649 | 0.46 | 3.83 | 0.44 | 0.31 |
| 19 | 215 | 75 | 89 | 257 | 17 | 653 | 0.45 | 3.54 | 0.41 | 0.3 |
| 20 | 223 | 74 | 96 | 253 | 15 | 661 | 0.46 | 4.4 | 0.42 | 0.32 |

[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




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

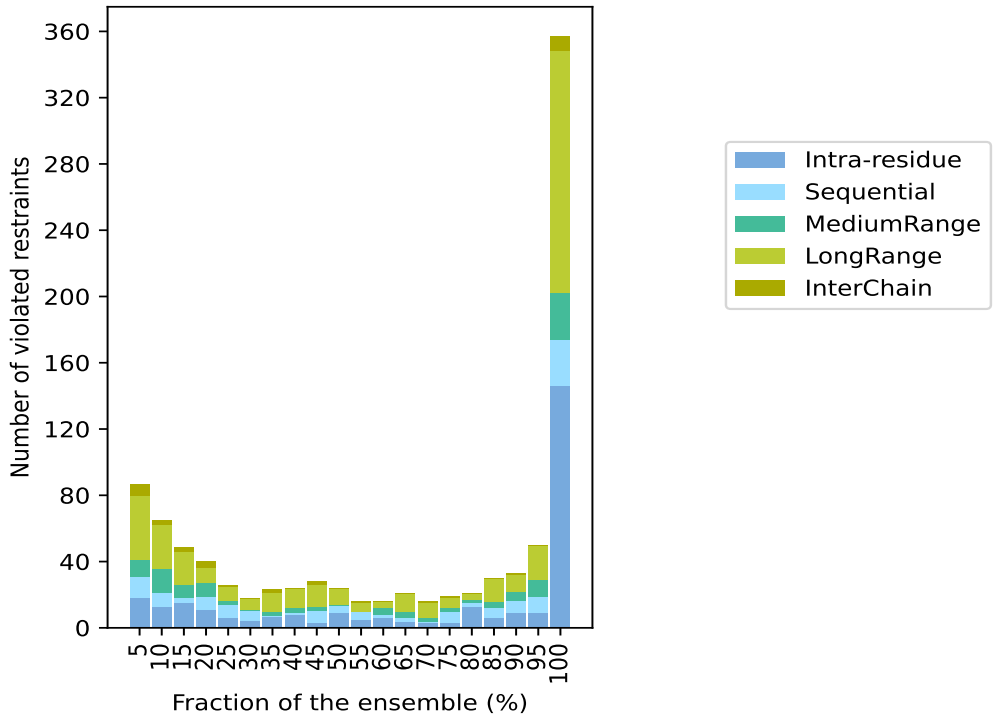
## 9.3 Distance violation statistics for the ensemble (i)

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, 3484(IR:1308, SQ:940, MR:568, LR:604, IC:64) 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] | % |
| 18 | 13 | 10 | 39 | 7 | 87 | 1 | 5.0 |
| 13 | 8 | 15 | 26 | 3 | 65 | 2 | 10.0 |
| 15 | 3 | 8 | 20 | 3 | 49 | 3 | 15.0 |
| 11 | 8 | 8 | 9 | 4 | 40 | 4 | 20.0 |
| 6 | 8 | 2 | 9 | 1 | 26 | 5 | 25.0 |
| 4 | 6 | 1 | 7 | 0 | 18 | 6 | 30.0 |
| 7 | 0 | 3 | 11 | 2 | 23 | 7 | 35.0 |
| 8 | 1 | 3 | 12 | 0 | 24 | 8 | 40.0 |
| 3 | 7 | 3 | 13 | 2 | 28 | 9 | 45.0 |
| 9 | 4 | 1 | 10 | 0 | 24 | 10 | 50.0 |
| 5 | 5 | 0 | 5 | 1 | 16 | 11 | 55.0 |
| 6 | 2 | 4 | 4 | 0 | 16 | 12 | 60.0 |
| 4 | 2 | 4 | 11 | 0 | 21 | 13 | 65.0 |
| 3 | 1 | 2 | 9 | 1 | 16 | 14 | 70.0 |
| 3 | 7 | 2 | 6 | 1 | 19 | 15 | 75.0 |
| 13 | 2 | 2 | 4 | 0 | 21 | 16 | 80.0 |
| 6 | 6 | 4 | 14 | 0 | 30 | 17 | 85.0 |
| 9 | 7 | 6 | 10 | 1 | 33 | 18 | 90.0 |
| 9 | 10 | 10 | 21 | 0 | 50 | 19 | 95.0 |
| 146 | 28 | 28 | 146 | 9 | 357 | 20 | 100.0 |

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

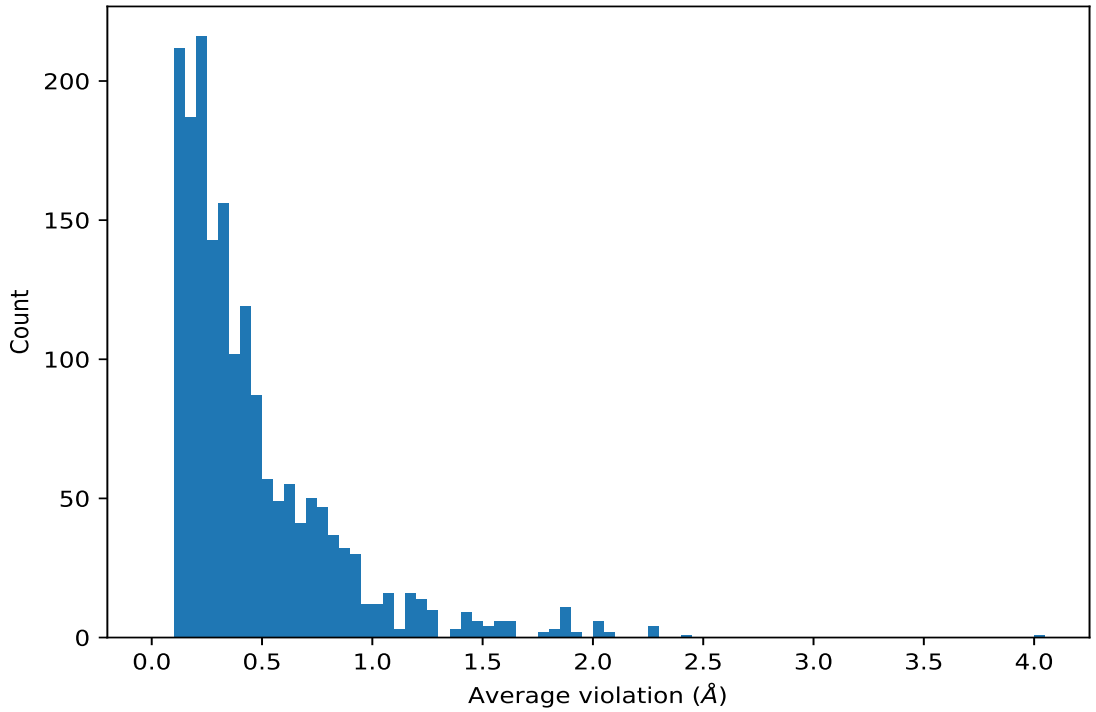
### 9.3.1 Bar graph : Distance violation statistics for the ensemble




## 9.4 Most violated distance restraints in the ensemble

### 9.4.1 Histogram : Distribution of mean distance violations

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




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

The following table provides the mean and the standard deviation of theviolation 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) |
|---|---|---|---|---|---|---|
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 20 | 4.0 | 0.85 | 3.76 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 20 | 2.4 | 0.53 | 2.17 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 20 | 2.26 | 0.04 | 2.26 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 20 | 2.26 | 0.04 | 2.26 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 20 | 2.25 | 0.11 | 2.26 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD13 | 20 | 2.25 | 0.11 | 2.26 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 20 | 2.09 | 0.38 | 2.13 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 20 | 2.05 | 1.11 | 2.06 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 20 | 2.03 | 0.14 | 2.02 |
| (4,315) | 1:56:A:ILE:HG21 | 1:6:A:LYS:HA | 20 | 2.03 | 0.14 | 2.02 |
| (4,315) | 1:56:A:ILE:HG22 | 1:6:A:LYS:HA | 20 | 2.03 | 0.14 | 2.02 |
| (4,315) | 1:56:A:ILE:HG22 | 1:38:A:LEU:HA | 20 | 2.03 | 0.14 | 2.02 |
| (2,1527) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 20 | 2.01 | 0.42 | 2.17 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 20 | 2.01 | 0.42 | 2.17 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 20 | 1.94 | 0.36 | 1.94 |
| (4,186) | 1:175:A:PHE:H | 2:201:A:NAD:H2A | 20 | 1.94 | 0.36 | 1.94 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 20 | 1.88 | 0.97 | 1.72 |
| (4,326) | 1:124:A:LEU:HD21 | 1:177:A:LYS:HE2 | 20 | 1.86 | 0.21 | 1.96 |
| (4,326) | 1:124:A:LEU:HD22 | 1:163:A:ASN:HB2 | 20 | 1.86 | 0.21 | 1.96 |
| (4,326) | 1:124:A:LEU:HD22 | 1:177:A:LYS:HE2 | 20 | 1.86 | 0.21 | 1.96 |
| (4,326) | 1:124:A:LEU:HD23 | 1:177:A:LYS:HE2 | 20 | 1.86 | 0.21 | 1.96 |
| (4,326) | 1:124:A:LEU:HD21 | 1:163:A:ASN:HB2 | 20 | 1.86 | 0.21 | 1.96 |
| (4,326) | 1:124:A:LEU:HD23 | 1:163:A:ASN:HB2 | 20 | 1.86 | 0.21 | 1.96 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 20 | 1.85 | 0.15 | 1.85 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG22 | 20 | 1.85 | 0.15 | 1.85 |
| (2,1802) | 1:53:A:LEU:HD13 | 1:74:A:ILE:HG23 | 20 | 1.85 | 0.15 | 1.85 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG21 | 20 | 1.85 | 0.15 | 1.85 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 20 | 1.79 | 0.06 | 1.8 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD13 | 20 | 1.79 | 0.06 | 1.8 |
| (4,441) | 1:56:A:ILE:HD11 | 1:38:A:LEU:HB2 | 20 | 1.58 | 0.16 | 1.59 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 20 | 1.58 | 0.16 | 1.59 |
| (4,441) | 1:56:A:ILE:HD11 | 1:6:A:LYS:HB3 | 20 | 1.58 | 0.16 | 1.59 |
| (4,441) | 1:56:A:ILE:HD12 | 1:38:A:LEU:HB2 | 20 | 1.58 | 0.16 | 1.59 |
| (4,441) | 1:56:A:ILE:HD12 | 1:6:A:LYS:HB3 | 20 | 1.58 | 0.16 | 1.59 |
| (4,441) | 1:56:A:ILE:HD13 | 1:6:A:LYS:HB3 | 20 | 1.58 | 0.16 | 1.59 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 20 | 1.5 | 0.23 | 1.53 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 20 | 1.5 | 0.23 | 1.53 |
| (2,3454) | 1:168:A:ILE:HD13 | 1:149:A:LYS:H | 20 | 1.5 | 0.23 | 1.53 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 20 | 1.48 | 0.04 | 1.48 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 20 | 1.48 | 0.04 | 1.48 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD12 | 20 | 1.48 | 0.04 | 1.48 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 20 | 1.46 | 0.05 | 1.45 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 20 | 1.46 | 0.05 | 1.45 |
| (2,1421) | 1:21:A:LEU:HD21 | 1:10:A:PHE:HE1 | 20 | 1.46 | 0.05 | 1.45 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 20 | 1.43 | 0.07 | 1.42 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG22 | 20 | 1.43 | 0.07 | 1.42 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 20 | 1.42 | 0.56 | 1.66 |
| (4,316) | 1:37:A:LEU:HD22 | 1:8:A:SER:HB2 | 20 | 1.42 | 0.56 | 1.66 |
| (4,316) | 1:37:A:LEU:HD23 | 1:23:A:GLY:HA3 | 20 | 1.42 | 0.56 | 1.66 |
| (4,316) | 1:37:A:LEU:HD21 | 1:8:A:SER:HB2 | 20 | 1.42 | 0.56 | 1.66 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 20 | 1.42 | 0.7 | 1.86 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 20 | 1.41 | 0.34 | 1.48 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 20 | 1.37 | 0.03 | 1.37 |
| (2,1530) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 20 | 1.37 | 0.03 | 1.37 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 20 | 1.28 | 0.07 | 1.29 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 20 | 1.28 | 0.07 | 1.29 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 20 | 1.28 | 0.23 | 1.31 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 20 | 1.28 | 0.23 | 1.31 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1487) | 1:168:A:ILE:HD13 | 1:149:A:LYS:H | 20 | 1.28 | 0.23 | 1.31 |
| (2,3498) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 20 | 1.26 | 0.42 | 1.42 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 20 | 1.26 | 0.42 | 1.42 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 20 | 1.25 | 0.3 | 1.14 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 20 | 1.25 | 0.3 | 1.14 |
| (2,1559) | 1:21:A:LEU:HD21 | 1:41:A:MET:HB2 | 20 | 1.25 | 0.3 | 1.14 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 20 | 1.24 | 0.04 | 1.25 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB1 | 20 | 1.24 | 0.13 | 1.21 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 20 | 1.24 | 0.13 | 1.21 |
| (2,3830) | 1:97:A:LEU:HD22 | 1:95:A:ALA:HB2 | 20 | 1.24 | 0.13 | 1.21 |
| (2,3830) | 1:97:A:LEU:HD23 | 1:95:A:ALA:HB2 | 20 | 1.24 | 0.13 | 1.21 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB3 | 20 | 1.24 | 0.13 | 1.21 |
| (2,3830) | 1:97:A:LEU:HD22 | 1:95:A:ALA:HB1 | 20 | 1.24 | 0.13 | 1.21 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 20 | 1.21 | 0.27 | 1.3 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 20 | 1.21 | 0.25 | 1.28 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 20 | 1.21 | 0.25 | 1.28 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD21 | 20 | 1.21 | 0.25 | 1.28 |
| (2,1783) | 1:44:A:LYS:HG3 | 1:21:A:LEU:HD22 | 20 | 1.21 | 0.25 | 1.28 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 20 | 1.2 | 0.07 | 1.18 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG22 | 20 | 1.2 | 0.07 | 1.18 |
| (2,1452) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 20 | 1.19 | 0.02 | 1.19 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 20 | 1.19 | 0.02 | 1.19 |
| (2,1452) | 1:38:A:LEU:HD11 | 1:38:A:LEU:H | 20 | 1.19 | 0.02 | 1.19 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 20 | 1.18 | 0.2 | 1.18 |
| (4,414) | 1:133:A:LYS:HB2 | 1:128:A:ILE:HG21 | 20 | 1.18 | 0.2 | 1.18 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 20 | 1.17 | 0.14 | 1.16 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG12 | 20 | 1.17 | 0.14 | 1.16 |
| (2,1260) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HG11 | 20 | 1.17 | 0.14 | 1.16 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 20 | 1.15 | 0.09 | 1.2 |
| (2,1843) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HB3 | 20 | 1.15 | 0.09 | 1.2 |
| (2,1843) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HB3 | 20 | 1.15 | 0.09 | 1.2 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 20 | 1.15 | 0.03 | 1.15 |
| (2,1806) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HB2 | 20 | 1.15 | 0.03 | 1.15 |
| (2,1806) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HB2 | 20 | 1.15 | 0.03 | 1.15 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 20 | 1.11 | 0.03 | 1.11 |
| (2,3501) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 20 | 1.11 | 0.03 | 1.11 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB1 | 20 | 1.09 | 0.13 | 1.06 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 20 | 1.09 | 0.13 | 1.06 |
| (2,1868) | 1:97:A:LEU:HD22 | 1:95:A:ALA:HB2 | 20 | 1.09 | 0.13 | 1.06 |
| (2,1868) | 1:97:A:LEU:HD23 | 1:95:A:ALA:HB2 | 20 | 1.09 | 0.13 | 1.06 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB3 | 20 | 1.09 | 0.13 | 1.06 |
| (2,1868) | 1:97:A:LEU:HD22 | 1:95:A:ALA:HB1 | 20 | 1.09 | 0.13 | 1.06 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 20 | 1.08 | 0.27 | 1.17 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 20 | 1.07 | 0.02 | 1.07 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 20 | 1.07 | 0.02 | 1.07 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 20 | 1.07 | 0.08 | 1.12 |
| (2,3807) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HB3 | 20 | 1.07 | 0.08 | 1.12 |
| (2,3807) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HB3 | 20 | 1.07 | 0.08 | 1.12 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 20 | 1.04 | 0.25 | 1.07 |
| (4,184) | 1:105:A:ASN:H | 1:136:A:MET:H | 20 | 1.04 | 0.25 | 1.07 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 20 | 1.04 | 0.25 | 1.08 |
| (4,202) | 1:173:A:ALA:HA | 1:145:A:SER:HB2 | 20 | 1.04 | 0.25 | 1.08 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 20 | 1.02 | 0.13 | 1.1 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 20 | 1.02 | 0.13 | 1.1 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG13 | 20 | 1.02 | 0.13 | 1.1 |
| (4,378) | 1:24:A:LEU:HA | 1:15:A:LEU:HB2 | 20 | 1.01 | 0.12 | 0.98 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 20 | 1.01 | 0.12 | 0.98 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 20 | 0.99 | 0.02 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 20 | 0.99 | 0.02 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 20 | 0.99 | 0.02 | 1.0 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 20 | 0.99 | 0.08 | 1.0 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 20 | 0.99 | 0.57 | 0.76 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 20 | 0.94 | 0.25 | 1.02 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 20 | 0.94 | 0.25 | 1.02 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD21 | 20 | 0.94 | 0.25 | 1.02 |
| (2,3749) | 1:44:A:LYS:HG3 | 1:21:A:LEU:HD22 | 20 | 0.94 | 0.25 | 1.02 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 20 | 0.94 | 0.04 | 0.94 |
| (2,816) | 1:53:A:LEU:HD21 | 1:53:A:LEU:H | 20 | 0.94 | 0.04 | 0.94 |
| (2,816) | 1:53:A:LEU:HD22 | 1:53:A:LEU:H | 20 | 0.94 | 0.04 | 0.94 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 20 | 0.93 | 0.21 | 1.01 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 20 | 0.92 | 0.03 | 0.92 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 20 | 0.92 | 0.03 | 0.92 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 20 | 0.92 | 0.03 | 0.92 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 20 | 0.92 | 0.03 | 0.92 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD21 | 20 | 0.92 | 0.1 | 0.93 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD22 | 20 | 0.92 | 0.1 | 0.93 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD12 | 20 | 0.92 | 0.1 | 0.93 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD13 | 20 | 0.92 | 0.1 | 0.93 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD23 | 20 | 0.92 | 0.1 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 20 | 0.9 | 0.19 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 20 | 0.9 | 0.19 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD11 | 20 | 0.9 | 0.19 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD13 | 20 | 0.9 | 0.19 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD13 | 20 | 0.9 | 0.19 | 0.93 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD13 | 20 | 0.9 | 0.19 | 0.93 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 20 | 0.9 | 0.03 | 0.9 |
| (2,3771) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HB2 | 20 | 0.9 | 0.03 | 0.9 |
| (2,3771) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HB2 | 20 | 0.9 | 0.03 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 20 | 0.89 | 0.03 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD22 | 20 | 0.89 | 0.03 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 20 | 0.89 | 0.03 | 0.9 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 20 | 0.88 | 0.06 | 0.9 |
| (2,1830) | 1:34:A:VAL:HG12 | 1:50:A:MET:HE2 | 20 | 0.88 | 0.22 | 0.94 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 20 | 0.88 | 0.22 | 0.94 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 20 | 0.88 | 0.22 | 0.94 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE1 | 20 | 0.88 | 0.22 | 0.94 |
| (2,1830) | 1:34:A:VAL:HG12 | 1:50:A:MET:HE1 | 20 | 0.88 | 0.22 | 0.94 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 20 | 0.87 | 0.17 | 0.89 |
| (2,1500) | 1:11:A:LEU:HD12 | 1:38:A:LEU:HA | 20 | 0.87 | 0.17 | 0.89 |
| (2,1495) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 20 | 0.85 | 0.1 | 0.86 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 20 | 0.85 | 0.1 | 0.86 |
| (2,1495) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 20 | 0.85 | 0.1 | 0.86 |
| (2,3421) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 20 | 0.85 | 0.02 | 0.85 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 20 | 0.85 | 0.02 | 0.85 |
| (2,3421) | 1:38:A:LEU:HD11 | 1:38:A:LEU:H | 20 | 0.85 | 0.02 | 0.85 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD23 | 20 | 0.85 | 0.24 | 0.9 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 20 | 0.85 | 0.24 | 0.9 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD22 | 20 | 0.85 | 0.24 | 0.9 |
| (4,36) | 1:76:A:ALA:H | 1:57:A:VAL:HG23 | 20 | 0.85 | 0.24 | 0.9 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 20 | 0.85 | 0.09 | 0.84 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD13 | 20 | 0.85 | 0.09 | 0.84 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD11 | 20 | 0.85 | 0.09 | 0.84 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 20 | 0.84 | 0.1 | 0.84 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD13 | 20 | 0.84 | 0.1 | 0.84 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD12 | 20 | 0.84 | 0.1 | 0.84 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 20 | 0.84 | 0.17 | 0.88 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD22 | 20 | 0.84 | 0.17 | 0.88 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD21 | 20 | 0.84 | 0.17 | 0.88 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 20 | 0.84 | 0.24 | 0.82 |
| (4,103) | 1:114:A:ILE:H | 1:123:A:HIS:HA | 20 | 0.84 | 0.24 | 0.82 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 20 | 0.83 | 0.16 | 0.9 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 20 | 0.83 | 0.08 | 0.83 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 20 | 0.83 | 0.05 | 0.82 |
| (2,1845) | 1:176:A:ILE:HB | 1:110:A:LEU:HD11 | 20 | 0.83 | 0.05 | 0.82 |
| (2,1845) | 1:110:A:LEU:HD13 | 1:176:A:ILE:HB | 20 | 0.83 | 0.05 | 0.82 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 20 | 0.82 | 0.02 | 0.82 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1856) | 1:22:A:ILE:HD12 | 1:14:A:VAL:HG23 | 20 | 0.82 | 0.23 | 0.76 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 20 | 0.82 | 0.23 | 0.76 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG23 | 20 | 0.82 | 0.23 | 0.76 |
| (2,1856) | 1:22:A:ILE:HD12 | 1:14:A:VAL:HG22 | 20 | 0.82 | 0.23 | 0.76 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG21 | 20 | 0.82 | 0.23 | 0.76 |
| (2,1856) | 1:22:A:ILE:HD13 | 1:14:A:VAL:HG21 | 20 | 0.82 | 0.23 | 0.76 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 20 | 0.81 | 0.12 | 0.81 |
| (4,329) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HA | 20 | 0.81 | 0.12 | 0.81 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 20 | 0.81 | 0.02 | 0.81 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG12 | 20 | 0.81 | 0.02 | 0.81 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 20 | 0.81 | 0.17 | 0.87 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG22 | 20 | 0.81 | 0.17 | 0.87 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 20 | 0.8 | 0.09 | 0.81 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 20 | 0.79 | 0.11 | 0.84 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 20 | 0.79 | 0.11 | 0.84 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 20 | 0.78 | 0.05 | 0.8 |
| (2,954) | 1:56:A:ILE:HG23 | 1:57:A:VAL:H | 20 | 0.78 | 0.05 | 0.8 |
| (2,954) | 1:56:A:ILE:HG21 | 1:57:A:VAL:H | 20 | 0.78 | 0.05 | 0.8 |
| (2,3462) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 20 | 0.77 | 0.1 | 0.78 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 20 | 0.77 | 0.1 | 0.78 |
| (2,3462) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 20 | 0.77 | 0.1 | 0.78 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 20 | 0.76 | 0.1 | 0.77 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 20 | 0.76 | 0.07 | 0.76 |
| (2,1473) | 1:110:A:LEU:HD13 | 1:110:A:LEU:H | 20 | 0.76 | 0.07 | 0.76 |
| (2,1473) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 20 | 0.76 | 0.07 | 0.76 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 20 | 0.76 | 0.09 | 0.74 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 20 | 0.76 | 0.01 | 0.75 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 20 | 0.75 | 0.02 | 0.75 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 20 | 0.74 | 0.21 | 0.82 |
| (4,244) | 1:51:A:GLU:HG2 | 1:67:A:PHE:HD1 | 20 | 0.74 | 0.21 | 0.82 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 20 | 0.74 | 0.23 | 0.66 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 20 | 0.74 | 0.23 | 0.66 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 20 | 0.74 | 0.07 | 0.75 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 20 | 0.74 | 0.07 | 0.75 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 20 | 0.74 | 0.08 | 0.73 |
| (2,1742) | 1:110:A:LEU:HD11 | 1:173:A:ALA:HA | 20 | 0.74 | 0.08 | 0.73 |
| (2,1742) | 1:110:A:LEU:HD13 | 1:173:A:ALA:HA | 20 | 0.74 | 0.08 | 0.73 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 20 | 0.73 | 0.06 | 0.71 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 20 | 0.73 | 0.36 | 0.75 |
| (4,7) | 1:65:A:PHE:HZ | 1:37:A:LEU:HD21 | 20 | 0.73 | 0.36 | 0.75 |
| (4,7) | 1:65:A:PHE:HZ | 1:37:A:LEU:HD23 | 20 | 0.73 | 0.36 | 0.75 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 20 | 0.73 | 0.29 | 0.73 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 20 | 0.73 | 0.29 | 0.73 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG21 | 20 | 0.73 | 0.29 | 0.73 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 20 | 0.72 | 0.24 | 0.72 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD12 | 20 | 0.72 | 0.24 | 0.72 |
| (2,1865) | 1:109:A:ILE:HD11 | 1:144:A:LEU:HD13 | 20 | 0.72 | 0.24 | 0.72 |
| (2,1865) | 1:109:A:ILE:HD11 | 1:144:A:LEU:HD11 | 20 | 0.72 | 0.24 | 0.72 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 20 | 0.72 | 0.01 | 0.72 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD23 | 20 | 0.72 | 0.01 | 0.72 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD22 | 20 | 0.72 | 0.01 | 0.72 |
| (4,431) | 1:13:A:LEU:HG | 1:13:A:LEU:HD12 | 20 | 0.72 | 0.01 | 0.72 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 20 | 0.72 | 0.16 | 0.78 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 20 | 0.71 | 0.57 | 0.5 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 20 | 0.7 | 0.2 | 0.72 |
| (4,204) | 1:173:A:ALA:HB1 | 1:111:A:LYS:HG3 | 20 | 0.7 | 0.2 | 0.72 |
| (4,204) | 1:173:A:ALA:HB1 | 1:111:A:LYS:HG2 | 20 | 0.7 | 0.2 | 0.72 |
| (4,204) | 1:173:A:ALA:HB2 | 1:111:A:LYS:HG2 | 20 | 0.7 | 0.2 | 0.72 |
| (4,204) | 1:173:A:ALA:HB3 | 1:111:A:LYS:HG3 | 20 | 0.7 | 0.2 | 0.72 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 20 | 0.7 | 0.03 | 0.69 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 20 | 0.7 | 0.17 | 0.77 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 20 | 0.7 | 0.31 | 0.58 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD3 | 20 | 0.7 | 0.31 | 0.58 |
| (4,167) | 1:34:A:VAL:H | 1:11:A:LEU:HB3 | 20 | 0.7 | 0.31 | 0.58 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 20 | 0.7 | 0.02 | 0.7 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 20 | 0.69 | 0.07 | 0.69 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 20 | 0.68 | 0.16 | 0.7 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 20 | 0.68 | 0.16 | 0.7 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 20 | 0.67 | 0.07 | 0.66 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD21 | 20 | 0.67 | 0.07 | 0.66 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD23 | 20 | 0.67 | 0.07 | 0.66 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 20 | 0.67 | 0.04 | 0.67 |
| (2,2784) | 1:53:A:LEU:HD21 | 1:53:A:LEU:H | 20 | 0.67 | 0.04 | 0.67 |
| (2,2784) | 1:53:A:LEU:HD22 | 1:53:A:LEU:H | 20 | 0.67 | 0.04 | 0.67 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 20 | 0.67 | 0.02 | 0.66 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 20 | 0.66 | 0.29 | 0.66 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 20 | 0.66 | 0.29 | 0.66 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG21 | 20 | 0.66 | 0.29 | 0.66 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 20 | 0.66 | 0.02 | 0.65 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 20 | 0.65 | 0.03 | 0.65 |
| (2,1297) | 1:57:A:VAL:HG13 | 1:67:A:PHE:HB3 | 20 | 0.65 | 0.03 | 0.65 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 20 | 0.64 | 0.02 | 0.64 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 20 | 0.64 | 0.03 | 0.63 |
| (2,3271) | 1:57:A:VAL:HG13 | 1:67:A:PHE:HB3 | 20 | 0.64 | 0.03 | 0.63 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 20 | 0.64 | 0.05 | 0.64 |
| (2,3813) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 20 | 0.64 | 0.19 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 20 | 0.64 | 0.19 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD11 | 20 | 0.64 | 0.19 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD13 | 20 | 0.64 | 0.19 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD13 | 20 | 0.64 | 0.19 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD13 | 20 | 0.64 | 0.19 | 0.67 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 20 | 0.64 | 0.18 | 0.72 |
| (2,1425) | 1:56:A:ILE:HG23 | 1:65:A:PHE:HD1 | 20 | 0.64 | 0.18 | 0.72 |
| (2,1425) | 1:56:A:ILE:HG21 | 1:65:A:PHE:HD1 | 20 | 0.64 | 0.18 | 0.72 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 20 | 0.63 | 0.14 | 0.64 |
| (2,3470) | 1:110:A:LEU:HD13 | 1:107:A:ASP:HA | 20 | 0.63 | 0.14 | 0.64 |
| (2,3470) | 1:110:A:LEU:HD12 | 1:107:A:ASP:HA | 20 | 0.63 | 0.14 | 0.64 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 20 | 0.63 | 0.06 | 0.64 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB2 | 20 | 0.63 | 0.2 | 0.67 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 20 | 0.63 | 0.2 | 0.67 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB3 | 20 | 0.63 | 0.2 | 0.67 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 20 | 0.63 | 0.04 | 0.63 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 20 | 0.63 | 0.07 | 0.64 |
| (4,437) | 1:178:A:VAL:HG23 | 1:177:A:LYS:HG2 | 20 | 0.63 | 0.07 | 0.64 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 20 | 0.61 | 0.05 | 0.61 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 20 | 0.61 | 0.14 | 0.66 |
| (4,15) | 1:177:A:LYS:H | 1:96:A:VAL:HG21 | 20 | 0.61 | 0.14 | 0.66 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD12 | 20 | 0.61 | 0.14 | 0.66 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD11 | 20 | 0.61 | 0.14 | 0.66 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 20 | 0.61 | 0.15 | 0.69 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 20 | 0.6 | 0.03 | 0.6 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 20 | 0.6 | 0.1 | 0.6 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 20 | 0.59 | 0.14 | 0.65 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 20 | 0.59 | 0.02 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HG | 20 | 0.59 | 0.02 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HG | 20 | 0.59 | 0.02 | 0.59 |
| (4,436) | 1:178:A:VAL:HG13 | 1:110:A:LEU:HB3 | 20 | 0.58 | 0.37 | 0.43 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 20 | 0.58 | 0.37 | 0.43 |
| (4,436) | 1:178:A:VAL:HG11 | 1:110:A:LEU:HB3 | 20 | 0.58 | 0.37 | 0.43 |
| (4,436) | 1:34:A:VAL:HG11 | 1:35:A:LYS:HG3 | 20 | 0.58 | 0.37 | 0.43 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 20 | 0.58 | 0.11 | 0.6 |
| (4,278) | 1:142:A:VAL:HG12 | 1:102:A:ALA:H | 20 | 0.58 | 0.11 | 0.6 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 20 | 0.58 | 0.06 | 0.6 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 20 | 0.57 | 0.14 | 0.57 |
| (4,303) | 1:110:A:LEU:HD13 | 1:107:A:ASP:HA | 20 | 0.57 | 0.14 | 0.57 |
| (4,303) | 1:110:A:LEU:HD12 | 1:107:A:ASP:HA | 20 | 0.57 | 0.14 | 0.57 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 20 | 0.56 | 0.03 | 0.57 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 20 | 0.56 | 0.03 | 0.57 |
| (2,1462) | 1:14:A:VAL:HG23 | 1:14:A:VAL:H | 20 | 0.56 | 0.03 | 0.57 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 20 | 0.55 | 0.2 | 0.57 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 20 | 0.54 | 0.02 | 0.55 |
| (4,449) | 1:74:A:ILE:HD11 | 1:57:A:VAL:HG23 | 20 | 0.54 | 0.04 | 0.54 |
| (4,449) | 1:74:A:ILE:HD12 | 1:11:A:LEU:HD23 | 20 | 0.54 | 0.04 | 0.54 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG23 | 20 | 0.54 | 0.04 | 0.54 |
| (4,449) | 1:57:A:VAL:HG21 | 1:74:A:ILE:HD11 | 20 | 0.54 | 0.04 | 0.54 |
| (4,449) | 1:74:A:ILE:HD11 | 1:11:A:LEU:HD21 | 20 | 0.54 | 0.04 | 0.54 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG21 | 20 | 0.54 | 0.04 | 0.54 |
| (4,449) | 1:74:A:ILE:HD12 | 1:11:A:LEU:HD21 | 20 | 0.54 | 0.04 | 0.54 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 20 | 0.54 | 0.04 | 0.55 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 20 | 0.54 | 0.04 | 0.55 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD13 | 20 | 0.54 | 0.04 | 0.55 |
| (4,368) | 1:20:A:ALA:HB3 | 1:22:A:ILE:HB | 20 | 0.53 | 0.08 | 0.53 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 20 | 0.53 | 0.08 | 0.53 |
| (4,368) | 1:20:A:ALA:HB1 | 1:22:A:ILE:HB | 20 | 0.53 | 0.08 | 0.53 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 20 | 0.53 | 0.02 | 0.54 |
| (2,1813) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HG | 20 | 0.53 | 0.02 | 0.54 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 20 | 0.51 | 0.09 | 0.52 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 20 | 0.51 | 0.09 | 0.52 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD11 | 20 | 0.51 | 0.06 | 0.5 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 20 | 0.51 | 0.06 | 0.5 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD12 | 20 | 0.51 | 0.06 | 0.5 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 20 | 0.51 | 0.11 | 0.5 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 20 | 0.5 | 0.06 | 0.49 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 20 | 0.5 | 0.06 | 0.49 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD12 | 20 | 0.5 | 0.06 | 0.49 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 20 | 0.49 | 0.04 | 0.48 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 20 | 0.49 | 0.04 | 0.48 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 20 | 0.49 | 0.04 | 0.48 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD11 | 20 | 0.49 | 0.04 | 0.48 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 20 | 0.49 | 0.04 | 0.48 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 20 | 0.49 | 0.04 | 0.48 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 20 | 0.49 | 0.15 | 0.5 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 20 | 0.48 | 0.01 | 0.49 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 20 | 0.48 | 0.02 | 0.48 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 20 | 0.48 | 0.05 | 0.48 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 20 | 0.48 | 0.1 | 0.46 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 20 | 0.48 | 0.1 | 0.46 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG22 | 20 | 0.48 | 0.08 | 0.47 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1859) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 20 | 0.48 | 0.08 | 0.47 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 20 | 0.48 | 0.08 | 0.47 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG23 | 20 | 0.48 | 0.08 | 0.47 |
| (2,1827) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HG | 20 | 0.47 | 0.06 | 0.46 |
| (2,1827) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HG | 20 | 0.47 | 0.06 | 0.46 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 20 | 0.47 | 0.06 | 0.46 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 20 | 0.47 | 0.05 | 0.46 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 20 | 0.47 | 0.05 | 0.46 |
| (2,1834) | 1:14:A:VAL:HG22 | 1:21:A:LEU:HG | 20 | 0.47 | 0.05 | 0.46 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 20 | 0.47 | 0.03 | 0.48 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 20 | 0.47 | 0.03 | 0.48 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 20 | 0.47 | 0.03 | 0.48 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 20 | 0.47 | 0.03 | 0.46 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 20 | 0.47 | 0.03 | 0.47 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 20 | 0.46 | 0.08 | 0.44 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 20 | 0.46 | 0.08 | 0.44 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD22 | 20 | 0.46 | 0.08 | 0.44 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 20 | 0.46 | 0.04 | 0.47 |
| (2,1872) | 1:168:A:ILE:HD11 | 1:168:A:ILE:HG13 | 20 | 0.46 | 0.04 | 0.47 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 20 | 0.46 | 0.03 | 0.45 |
| (2,3676) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 20 | 0.46 | 0.03 | 0.45 |
| (2,3676) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 20 | 0.46 | 0.03 | 0.45 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 20 | 0.46 | 0.17 | 0.45 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 20 | 0.46 | 0.17 | 0.45 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 20 | 0.46 | 0.01 | 0.46 |
| (2,1821) | 1:143:A:VAL:HG21 | 1:143:A:VAL:HB | 20 | 0.46 | 0.01 | 0.46 |
| (2,1821) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 20 | 0.46 | 0.01 | 0.46 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 20 | 0.46 | 0.06 | 0.47 |
| (2,1820) | 1:142:A:VAL:HG11 | 1:142:A:VAL:HB | 20 | 0.46 | 0.06 | 0.47 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 20 | 0.45 | 0.04 | 0.46 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 20 | 0.45 | 0.04 | 0.46 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD11 | 20 | 0.45 | 0.04 | 0.46 |
| (2,1744) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HA | 20 | 0.45 | 0.02 | 0.44 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 20 | 0.45 | 0.02 | 0.44 |
| (2,1744) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 20 | 0.45 | 0.02 | 0.44 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 20 | 0.45 | 0.22 | 0.36 |
| (2,1869) | 1:97:A:LEU:HD23 | 1:96:A:VAL:HB | 20 | 0.45 | 0.22 | 0.36 |
| (2,1869) | 1:97:A:LEU:HD22 | 1:96:A:VAL:HB | 20 | 0.45 | 0.22 | 0.36 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 20 | 0.45 | 0.01 | 0.45 |
| (2,3782) | 1:143:A:VAL:HG21 | 1:143:A:VAL:HB | 20 | 0.45 | 0.01 | 0.45 |
| (2,3782) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 20 | 0.45 | 0.01 | 0.45 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 20 | 0.45 | 0.11 | 0.45 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 20 | 0.44 | 0.02 | 0.44 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 20 | 0.44 | 0.06 | 0.44 |
| (2,175) | 1:53:A:LEU:HD21 | 1:56:A:ILE:H | 20 | 0.44 | 0.06 | 0.44 |
| (2,175) | 1:53:A:LEU:HD22 | 1:56:A:ILE:H | 20 | 0.44 | 0.06 | 0.44 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 20 | 0.44 | 0.02 | 0.44 |
| (2,3411) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 20 | 0.44 | 0.02 | 0.44 |
| (2,3411) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 20 | 0.44 | 0.02 | 0.44 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 20 | 0.44 | 0.05 | 0.44 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 20 | 0.44 | 0.09 | 0.45 |
| (2,1407) | 1:95:A:ALA:HB3 | 1:95:A:ALA:H | 20 | 0.44 | 0.09 | 0.45 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 20 | 0.44 | 0.07 | 0.45 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD21 | 20 | 0.43 | 0.06 | 0.44 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD22 | 20 | 0.43 | 0.06 | 0.44 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 20 | 0.43 | 0.06 | 0.44 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD21 | 20 | 0.43 | 0.06 | 0.44 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 20 | 0.43 | 0.05 | 0.45 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 20 | 0.43 | 0.05 | 0.45 |
| (4,447) | 1:53:A:LEU:HD12 | 1:11:A:LEU:HD23 | 20 | 0.43 | 0.05 | 0.45 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD11 | 20 | 0.43 | 0.05 | 0.45 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 20 | 0.43 | 0.02 | 0.43 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 20 | 0.43 | 0.02 | 0.43 |
| (2,3798) | 1:48:A:ILE:HD11 | 1:48:A:ILE:HG13 | 20 | 0.43 | 0.02 | 0.43 |
| (2,3399) | 1:21:A:LEU:HD13 | 1:21:A:LEU:H | 20 | 0.43 | 0.09 | 0.46 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 20 | 0.43 | 0.09 | 0.46 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 20 | 0.43 | 0.06 | 0.44 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 20 | 0.43 | 0.06 | 0.44 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG22 | 20 | 0.43 | 0.06 | 0.44 |
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 20 | 0.43 | 0.05 | 0.44 |
| (2,1819) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HG | 20 | 0.43 | 0.05 | 0.44 |
| (2,1819) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HG | 20 | 0.43 | 0.05 | 0.44 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 20 | 0.42 | 0.07 | 0.44 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG23 | 20 | 0.42 | 0.07 | 0.44 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 20 | 0.42 | 0.09 | 0.43 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 20 | 0.42 | 0.09 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 20 | 0.42 | 0.01 | 0.42 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 20 | 0.42 | 0.04 | 0.42 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 20 | 0.41 | 0.08 | 0.44 |
| (4,446) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HG | 20 | 0.41 | 0.08 | 0.44 |
| (4,446) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HG | 20 | 0.41 | 0.08 | 0.44 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD11 | 20 | 0.41 | 0.08 | 0.44 |
| (4,446) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HG | 20 | 0.41 | 0.08 | 0.44 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 20 | 0.41 | 0.04 | 0.4 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 20 | 0.41 | 0.11 | 0.48 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 20 | 0.41 | 0.18 | 0.4 |
| (4,259) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 20 | 0.41 | 0.18 | 0.4 |
| (4,259) | 1:117:A:MET:HE3 | 2:201:A:NAD:H2A | 20 | 0.41 | 0.18 | 0.4 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 20 | 0.41 | 0.02 | 0.42 |
| (2,3544) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 20 | 0.41 | 0.02 | 0.42 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 20 | 0.41 | 0.11 | 0.42 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 20 | 0.41 | 0.11 | 0.42 |
| (2,1849) | 1:15:A:LEU:HD13 | 1:74:A:ILE:HD11 | 20 | 0.41 | 0.11 | 0.42 |
| (2,1849) | 1:15:A:LEU:HD11 | 1:74:A:ILE:HD12 | 20 | 0.41 | 0.11 | 0.42 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 20 | 0.4 | 0.04 | 0.41 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 20 | 0.4 | 0.04 | 0.41 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD23 | 20 | 0.4 | 0.04 | 0.41 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 20 | 0.4 | 0.04 | 0.41 |
| (2,3833) | 1:168:A:ILE:HD11 | 1:168:A:ILE:HG13 | 20 | 0.4 | 0.04 | 0.41 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 20 | 0.4 | 0.04 | 0.4 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 20 | 0.4 | 0.02 | 0.4 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 20 | 0.4 | 0.02 | 0.4 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 20 | 0.4 | 0.05 | 0.42 |
| (2,1699) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 20 | 0.39 | 0.01 | 0.4 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 20 | 0.39 | 0.01 | 0.4 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB2 | 20 | 0.39 | 0.01 | 0.4 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 20 | 0.39 | 0.08 | 0.4 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 20 | 0.39 | 0.05 | 0.38 |
| (2,1793) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HB2 | 20 | 0.39 | 0.05 | 0.38 |
| (2,3666) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 20 | 0.39 | 0.01 | 0.39 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 20 | 0.39 | 0.01 | 0.39 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB2 | 20 | 0.39 | 0.01 | 0.39 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 20 | 0.39 | 0.23 | 0.22 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 20 | 0.39 | 0.01 | 0.39 |
| (2,1221) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 20 | 0.39 | 0.01 | 0.39 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 20 | 0.39 | 0.03 | 0.4 |
| (2,3677) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HA | 20 | 0.39 | 0.03 | 0.4 |
| (2,3677) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HA | 20 | 0.39 | 0.03 | 0.4 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 20 | 0.38 | 0.07 | 0.4 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD21 | 20 | 0.37 | 0.04 | 0.36 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 20 | 0.37 | 0.04 | 0.36 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD23 | 20 | 0.37 | 0.04 | 0.36 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 20 | 0.37 | 0.04 | 0.38 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG22 | 20 | 0.37 | 0.04 | 0.38 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 20 | 0.36 | 0.02 | 0.36 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 20 | 0.36 | 0.02 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD12 | 20 | 0.36 | 0.02 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HB2 | 20 | 0.36 | 0.01 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 20 | 0.36 | 0.01 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 20 | 0.36 | 0.01 | 0.36 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 20 | 0.36 | 0.02 | 0.36 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 20 | 0.36 | 0.02 | 0.36 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD21 | 20 | 0.36 | 0.02 | 0.36 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 20 | 0.35 | 0.04 | 0.35 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 20 | 0.35 | 0.04 | 0.35 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD12 | 20 | 0.35 | 0.04 | 0.35 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 20 | 0.35 | 0.04 | 0.36 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 20 | 0.35 | 0.06 | 0.36 |
| (2,3781) | 1:142:A:VAL:HG11 | 1:142:A:VAL:HB | 20 | 0.35 | 0.06 | 0.36 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 20 | 0.35 | 0.02 | 0.35 |
| (2,1692) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 20 | 0.35 | 0.02 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 20 | 0.35 | 0.01 | 0.35 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 20 | 0.34 | 0.03 | 0.36 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 20 | 0.34 | 0.03 | 0.36 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 20 | 0.34 | 0.01 | 0.34 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 20 | 0.34 | 0.01 | 0.34 |
| (2,3783) | 1:143:A:VAL:HG11 | 1:143:A:VAL:HB | 20 | 0.34 | 0.01 | 0.34 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 20 | 0.34 | 0.04 | 0.32 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 20 | 0.34 | 0.04 | 0.32 |
| (2,1838) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 20 | 0.34 | 0.03 | 0.34 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 20 | 0.34 | 0.03 | 0.34 |
| (2,1838) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 20 | 0.34 | 0.03 | 0.34 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 20 | 0.34 | 0.07 | 0.32 |
| (2,3439) | 1:110:A:LEU:HD13 | 1:110:A:LEU:H | 20 | 0.34 | 0.07 | 0.32 |
| (2,3439) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 20 | 0.34 | 0.07 | 0.32 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 20 | 0.34 | 0.09 | 0.35 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 20 | 0.33 | 0.11 | 0.35 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD12 | 20 | 0.33 | 0.11 | 0.35 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 20 | 0.33 | 0.05 | 0.34 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 20 | 0.33 | 0.02 | 0.33 |
| (2,1532) | 1:34:A:VAL:HG13 | 1:34:A:VAL:HA | 20 | 0.33 | 0.02 | 0.34 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 20 | 0.33 | 0.02 | 0.34 |
| (2,1201) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 20 | 0.33 | 0.02 | 0.33 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 20 | 0.33 | 0.02 | 0.33 |
| (2,1201) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 20 | 0.33 | 0.02 | 0.33 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 20 | 0.33 | 0.04 | 0.32 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 20 | 0.33 | 0.04 | 0.32 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 20 | 0.33 | 0.03 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 20 | 0.33 | 0.04 | 0.31 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 20 | 0.33 | 0.02 | 0.32 |
| (2,1832) | 1:53:A:LEU:HD21 | 1:56:A:ILE:HB | 20 | 0.33 | 0.02 | 0.32 |
| (2,1832) | 1:53:A:LEU:HD22 | 1:56:A:ILE:HB | 20 | 0.33 | 0.02 | 0.32 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 20 | 0.33 | 0.05 | 0.32 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 20 | 0.33 | 0.05 | 0.32 |
| (2,3387) | 1:21:A:LEU:HD21 | 1:10:A:PHE:HE1 | 20 | 0.33 | 0.05 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 20 | 0.33 | 0.01 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 20 | 0.33 | 0.01 | 0.32 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 20 | 0.32 | 0.04 | 0.33 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 20 | 0.32 | 0.09 | 0.36 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 20 | 0.32 | 0.01 | 0.32 |
| (2,3196) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 20 | 0.32 | 0.01 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD22 | 20 | 0.32 | 0.02 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 20 | 0.32 | 0.02 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD23 | 20 | 0.32 | 0.02 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 20 | 0.32 | 0.02 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD22 | 20 | 0.32 | 0.02 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD21 | 20 | 0.32 | 0.02 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD23 | 20 | 0.32 | 0.02 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD21 | 20 | 0.32 | 0.02 | 0.32 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 20 | 0.32 | 0.02 | 0.32 |
| (2,3659) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 20 | 0.32 | 0.02 | 0.32 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 20 | 0.32 | 0.02 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 20 | 0.32 | 0.01 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 20 | 0.32 | 0.01 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB2 | 1:28:A:ALA:HA | 20 | 0.32 | 0.01 | 0.32 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 20 | 0.32 | 0.02 | 0.32 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 20 | 0.32 | 0.02 | 0.32 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 20 | 0.32 | 0.02 | 0.32 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD21 | 20 | 0.32 | 0.02 | 0.32 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 20 | 0.31 | 0.06 | 0.3 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 20 | 0.31 | 0.06 | 0.3 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD12 | 20 | 0.31 | 0.06 | 0.3 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 20 | 0.31 | 0.01 | 0.31 |
| (2,1395) | 1:39:A:ALA:HB3 | 1:40:A:LYS:H | 20 | 0.31 | 0.01 | 0.31 |
| (2,3175) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 20 | 0.31 | 0.02 | 0.31 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 20 | 0.31 | 0.02 | 0.31 |
| (2,3175) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 20 | 0.31 | 0.02 | 0.31 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 20 | 0.31 | 0.01 | 0.32 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 20 | 0.31 | 0.04 | 0.33 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 20 | 0.31 | 0.04 | 0.33 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD13 | 20 | 0.31 | 0.04 | 0.33 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 20 | 0.31 | 0.06 | 0.28 |
| (2,3769) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 20 | 0.31 | 0.06 | 0.28 |
| (2,3769) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HB | 20 | 0.31 | 0.06 | 0.28 |
| (2,1874) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 20 | 0.31 | 0.06 | 0.31 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 20 | 0.31 | 0.06 | 0.31 |
| (2,1874) | 1:168:A:ILE:HD12 | 1:171:A:VAL:HG13 | 20 | 0.31 | 0.06 | 0.31 |
| (2,1874) | 1:168:A:ILE:HD12 | 1:171:A:VAL:HG11 | 20 | 0.31 | 0.06 | 0.31 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 20 | 0.31 | 0.04 | 0.31 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 20 | 0.31 | 0.03 | 0.32 |
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 20 | 0.31 | 0.03 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 20 | 0.31 | 0.03 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HG12 | 20 | 0.31 | 0.03 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG22 | 1:56:A:ILE:HG12 | 20 | 0.31 | 0.03 | 0.32 |
| (2,1858) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HD11 | 20 | 0.3 | 0.03 | 0.3 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 20 | 0.3 | 0.03 | 0.3 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 20 | 0.3 | 0.03 | 0.3 |
| (2,1858) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HD11 | 20 | 0.3 | 0.03 | 0.3 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 20 | 0.3 | 0.01 | 0.31 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 20 | 0.3 | 0.1 | 0.26 |
| (2,1435) | 1:15:A:LEU:HD22 | 1:15:A:LEU:H | 20 | 0.3 | 0.1 | 0.26 |
| (2,1435) | 1:15:A:LEU:HD23 | 1:15:A:LEU:H | 20 | 0.3 | 0.1 | 0.26 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 20 | 0.3 | 0.02 | 0.3 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG12 | 20 | 0.3 | 0.02 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 20 | 0.3 | 0.02 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 20 | 0.3 | 0.02 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG23 | 1:19:A:PRO:HA | 20 | 0.3 | 0.02 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 20 | 0.3 | 0.01 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 20 | 0.3 | 0.01 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB2 | 1:28:A:ALA:HA | 20 | 0.3 | 0.01 | 0.3 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 20 | 0.3 | 0.07 | 0.28 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 20 | 0.3 | 0.07 | 0.28 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 20 | 0.3 | 0.07 | 0.28 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 20 | 0.3 | 0.03 | 0.29 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 20 | 0.3 | 0.01 | 0.3 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 20 | 0.3 | 0.02 | 0.3 |
| (2,1573) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 20 | 0.3 | 0.02 | 0.3 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 20 | 0.3 | 0.02 | 0.29 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 20 | 0.3 | 0.05 | 0.31 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 20 | 0.29 | 0.01 | 0.29 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 20 | 0.29 | 0.01 | 0.29 |
| (2,1822) | 1:143:A:VAL:HG11 | 1:143:A:VAL:HB | 20 | 0.29 | 0.01 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 20 | 0.29 | 0.02 | 0.28 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 20 | 0.29 | 0.04 | 0.29 |
| (4,451) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG12 | 20 | 0.29 | 0.04 | 0.29 |
| (4,451) | 1:168:A:ILE:HD11 | 1:168:A:ILE:HG12 | 20 | 0.29 | 0.04 | 0.29 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 20 | 0.28 | 0.02 | 0.28 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 20 | 0.28 | 0.01 | 0.28 |
| (4,426) | 1:53:A:LEU:HD13 | 1:37:A:LEU:HG | 20 | 0.28 | 0.01 | 0.28 |
| (2,1301) | 1:34:A:VAL:HG13 | 1:38:A:LEU:H | 20 | 0.28 | 0.09 | 0.27 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 20 | 0.28 | 0.09 | 0.27 |
| (2,1301) | 1:34:A:VAL:HG12 | 1:38:A:LEU:H | 20 | 0.28 | 0.09 | 0.27 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 20 | 0.28 | 0.06 | 0.3 |
| (2,3826) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB3 | 20 | 0.28 | 0.06 | 0.3 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG22 | 20 | 0.28 | 0.08 | 0.27 |
| (2,3821) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 20 | 0.28 | 0.08 | 0.27 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 20 | 0.28 | 0.08 | 0.27 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG23 | 20 | 0.28 | 0.08 | 0.27 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 20 | 0.28 | 0.04 | 0.28 |
| (4,395) | 1:56:A:ILE:HG22 | 1:56:A:ILE:HA | 20 | 0.28 | 0.04 | 0.28 |
| (4,395) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HA | 20 | 0.28 | 0.04 | 0.28 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 20 | 0.28 | 0.02 | 0.27 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 20 | 0.28 | 0.01 | 0.28 |
| (2,1796) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD11 | 20 | 0.27 | 0.04 | 0.28 |
| (2,1796) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD12 | 20 | 0.27 | 0.04 | 0.28 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 20 | 0.27 | 0.04 | 0.28 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 20 | 0.27 | 0.04 | 0.28 |
| (2,1796) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD11 | 20 | 0.27 | 0.04 | 0.28 |
| (2,1796) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD12 | 20 | 0.27 | 0.04 | 0.28 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 20 | 0.27 | 0.06 | 0.24 |
| (2,1804) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 20 | 0.27 | 0.06 | 0.24 |
| (2,1804) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HB | 20 | 0.27 | 0.06 | 0.24 |
| (2,1857) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 20 | 0.27 | 0.04 | 0.27 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 20 | 0.27 | 0.04 | 0.27 |
| (2,1857) | 1:151:A:MET:HE2 | 1:171:A:VAL:HG12 | 20 | 0.27 | 0.04 | 0.27 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 20 | 0.27 | 0.03 | 0.28 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 20 | 0.27 | 0.02 | 0.28 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 20 | 0.27 | 0.05 | 0.26 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 20 | 0.27 | 0.05 | 0.26 |
| (2,3795) | 1:14:A:VAL:HG22 | 1:21:A:LEU:HG | 20 | 0.27 | 0.05 | 0.26 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 20 | 0.26 | 0.06 | 0.25 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 20 | 0.26 | 0.02 | 0.26 |
| (2,1576) | 1:22:A:ILE:HG21 | 1:22:A:ILE:HA | 20 | 0.26 | 0.02 | 0.26 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 20 | 0.26 | 0.04 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 20 | 0.26 | 0.04 | 0.25 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE1 | 20 | 0.26 | 0.04 | 0.25 |
| (2,2041) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 20 | 0.26 | 0.03 | 0.26 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 20 | 0.26 | 0.03 | 0.26 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 20 | 0.26 | 0.03 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 20 | 0.26 | 0.03 | 0.25 |
| (2,1709) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 20 | 0.26 | 0.03 | 0.25 |
| (2,1709) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 20 | 0.26 | 0.03 | 0.25 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 20 | 0.26 | 0.03 | 0.26 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD22 | 20 | 0.26 | 0.03 | 0.26 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 20 | 0.26 | 0.03 | 0.26 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 20 | 0.26 | 0.03 | 0.25 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 20 | 0.26 | 0.03 | 0.25 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 20 | 0.26 | 0.07 | 0.24 |
| (4,439) | 1:176:A:ILE:HG22 | 1:109:A:ILE:HB | 20 | 0.26 | 0.07 | 0.24 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 20 | 0.25 | 0.06 | 0.26 |
| (2,1863) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB3 | 20 | 0.25 | 0.06 | 0.26 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 20 | 0.25 | 0.05 | 0.25 |
| (2,3809) | 1:176:A:ILE:HB | 1:110:A:LEU:HD11 | 20 | 0.25 | 0.05 | 0.25 |
| (2,3809) | 1:110:A:LEU:HD13 | 1:176:A:ILE:HB | 20 | 0.25 | 0.05 | 0.25 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 20 | 0.25 | 0.06 | 0.23 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 20 | 0.25 | 0.06 | 0.23 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 20 | 0.25 | 0.06 | 0.23 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 20 | 0.25 | 0.02 | 0.24 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 20 | 0.25 | 0.01 | 0.24 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 20 | 0.24 | 0.02 | 0.25 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 20 | 0.24 | 0.02 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 20 | 0.24 | 0.02 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG22 | 20 | 0.24 | 0.02 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG23 | 1:14:A:VAL:HG21 | 20 | 0.24 | 0.02 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 20 | 0.24 | 0.06 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 20 | 0.24 | 0.06 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD12 | 1:171:A:VAL:HG13 | 20 | 0.24 | 0.06 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD12 | 1:171:A:VAL:HG11 | 20 | 0.24 | 0.06 | 0.24 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 20 | 0.24 | 0.05 | 0.23 |
| (2,3759) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HB2 | 20 | 0.24 | 0.05 | 0.23 |
| (2,1844) | 1:110:A:LEU:HD23 | 1:110:A:LEU:HB3 | 20 | 0.24 | 0.03 | 0.25 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 20 | 0.24 | 0.03 | 0.25 |
| (2,1844) | 1:110:A:LEU:HD22 | 1:110:A:LEU:HB3 | 20 | 0.24 | 0.03 | 0.25 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 20 | 0.24 | 0.03 | 0.24 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 20 | 0.24 | 0.03 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3710) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HA | 20 | 0.24 | 0.03 | 0.24 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 20 | 0.24 | 0.05 | 0.24 |
| (2,1810) | 1:21:A:LEU:HD12 | 1:21:A:LEU:HB3 | 20 | 0.24 | 0.05 | 0.25 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 20 | 0.24 | 0.05 | 0.25 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 20 | 0.23 | 0.04 | 0.24 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 20 | 0.23 | 0.01 | 0.23 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 20 | 0.23 | 0.05 | 0.24 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 20 | 0.23 | 0.02 | 0.23 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 20 | 0.23 | 0.03 | 0.24 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 20 | 0.23 | 0.05 | 0.24 |
| (2,3800) | 1:56:A:ILE:HD11 | 1:56:A:ILE:HG12 | 20 | 0.23 | 0.02 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 20 | 0.23 | 0.02 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD12 | 1:56:A:ILE:HG12 | 20 | 0.23 | 0.02 | 0.22 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 20 | 0.23 | 0.02 | 0.23 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 20 | 0.23 | 0.03 | 0.23 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 20 | 0.23 | 0.04 | 0.24 |
| (2,3424) | 1:165:A:VAL:HG23 | 2:201:A:NAD:H5N | 20 | 0.23 | 0.04 | 0.24 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 20 | 0.22 | 0.03 | 0.22 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 20 | 0.22 | 0.04 | 0.21 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 20 | 0.22 | 0.04 | 0.21 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE1 | 20 | 0.22 | 0.04 | 0.21 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 20 | 0.22 | 0.02 | 0.22 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 20 | 0.22 | 0.02 | 0.22 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 20 | 0.22 | 0.06 | 0.2 |
| (2,1861) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 20 | 0.22 | 0.06 | 0.2 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD11 | 20 | 0.22 | 0.06 | 0.2 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 20 | 0.22 | 0.01 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 20 | 0.22 | 0.02 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 20 | 0.22 | 0.02 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG22 | 20 | 0.22 | 0.02 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG23 | 1:14:A:VAL:HG21 | 20 | 0.22 | 0.02 | 0.22 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 20 | 0.22 | 0.02 | 0.21 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 20 | 0.22 | 0.01 | 0.22 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 20 | 0.22 | 0.02 | 0.22 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 20 | 0.22 | 0.02 | 0.22 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 20 | 0.22 | 0.04 | 0.22 |
| (2,1455) | 1:165:A:VAL:HG23 | 2:201:A:NAD:H5N | 20 | 0.22 | 0.04 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 20 | 0.22 | 0.01 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 20 | 0.22 | 0.01 | 0.22 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 20 | 0.21 | 0.06 | 0.19 |
| (2,3824) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 20 | 0.21 | 0.06 | 0.19 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD11 | 20 | 0.21 | 0.06 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 20 | 0.21 | 0.01 | 0.21 |
| (2,3841) | 1:76:A:ALA:HB1 | 1:76:A:ALA:H | 20 | 0.21 | 0.03 | 0.2 |
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 20 | 0.21 | 0.03 | 0.2 |
| (2,3841) | 1:76:A:ALA:HB3 | 1:76:A:ALA:H | 20 | 0.21 | 0.03 | 0.2 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 20 | 0.21 | 0.02 | 0.21 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 20 | 0.21 | 0.01 | 0.21 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 20 | 0.21 | 0.02 | 0.21 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 20 | 0.21 | 0.02 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 20 | 0.21 | 0.02 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG23 | 1:19:A:PRO:HA | 20 | 0.21 | 0.02 | 0.2 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 20 | 0.21 | 0.03 | 0.21 |
| (2,1524) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 20 | 0.21 | 0.03 | 0.21 |
| (2,1524) | 1:82:A:VAL:HG12 | 1:82:A:VAL:HA | 20 | 0.21 | 0.03 | 0.21 |
| (2,1524) | 1:82:A:VAL:HG13 | 1:82:A:VAL:HA | 20 | 0.21 | 0.03 | 0.21 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 20 | 0.21 | 0.04 | 0.21 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 20 | 0.2 | 0.01 | 0.2 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 20 | 0.2 | 0.02 | 0.2 |
| (2,1800) | 1:53:A:LEU:HD13 | 1:37:A:LEU:HG | 20 | 0.2 | 0.02 | 0.2 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 20 | 0.2 | 0.03 | 0.21 |
| (4,452) | 1:59:A:THR:HB | 1:59:A:THR:HG22 | 20 | 0.2 | 0.03 | 0.21 |
| (2,3819) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 20 | 0.2 | 0.04 | 0.2 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 20 | 0.2 | 0.04 | 0.2 |
| (2,3819) | 1:151:A:MET:HE2 | 1:171:A:VAL:HG12 | 20 | 0.2 | 0.04 | 0.2 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 20 | 0.2 | 0.03 | 0.21 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 20 | 0.2 | 0.03 | 0.21 |
| (2,3495) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 20 | 0.2 | 0.03 | 0.21 |
| (2,3495) | 1:82:A:VAL:HG12 | 1:82:A:VAL:HA | 20 | 0.2 | 0.03 | 0.21 |
| (2,3495) | 1:82:A:VAL:HG13 | 1:82:A:VAL:HA | 20 | 0.2 | 0.03 | 0.21 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 20 | 0.2 | 0.03 | 0.2 |
| (2,1194) | 1:176:A:ILE:HD12 | 1:114:A:ILE:HD13 | 20 | 0.2 | 0.03 | 0.2 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 20 | 0.2 | 0.02 | 0.21 |
| (2,3503) | 1:34:A:VAL:HG13 | 1:34:A:VAL:HA | 20 | 0.2 | 0.02 | 0.2 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 20 | 0.2 | 0.02 | 0.2 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 20 | 0.2 | 0.06 | 0.18 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 20 | 0.2 | 0.06 | 0.18 |
| (2,3794) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HB | 20 | 0.2 | 0.06 | 0.18 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 20 | 0.2 | 0.02 | 0.2 |
| (2,3547) | 1:22:A:ILE:HG21 | 1:22:A:ILE:HA | 20 | 0.2 | 0.02 | 0.2 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 20 | 0.2 | 0.03 | 0.21 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 20 | 0.2 | 0.01 | 0.2 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 20 | 0.19 | 0.02 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 20 | 0.19 | 0.01 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 20 | 0.19 | 0.02 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 20 | 0.19 | 0.0 | 0.19 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 20 | 0.18 | 0.02 | 0.18 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 20 | 0.18 | 0.02 | 0.18 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD12 | 20 | 0.18 | 0.02 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 20 | 0.18 | 0.01 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG22 | 1:96:A:VAL:HA | 20 | 0.18 | 0.01 | 0.18 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 20 | 0.18 | 0.02 | 0.18 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 20 | 0.18 | 0.01 | 0.18 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 20 | 0.18 | 0.02 | 0.18 |
| (2,3793) | 1:53:A:LEU:HD21 | 1:56:A:ILE:HB | 20 | 0.18 | 0.02 | 0.18 |
| (2,3793) | 1:53:A:LEU:HD22 | 1:56:A:ILE:HB | 20 | 0.18 | 0.02 | 0.18 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 20 | 0.18 | 0.02 | 0.17 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD22 | 20 | 0.17 | 0.02 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 20 | 0.17 | 0.02 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD23 | 20 | 0.17 | 0.02 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 20 | 0.17 | 0.02 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD22 | 20 | 0.17 | 0.02 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD21 | 20 | 0.17 | 0.02 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD23 | 20 | 0.17 | 0.02 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD21 | 20 | 0.17 | 0.02 | 0.18 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 20 | 0.17 | 0.01 | 0.17 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 20 | 0.17 | 0.03 | 0.17 |
| (2,3167) | 1:176:A:ILE:HD12 | 1:114:A:ILE:HD13 | 20 | 0.17 | 0.03 | 0.17 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 20 | 0.16 | 0.02 | 0.16 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 20 | 0.16 | 0.03 | 0.15 |
| (2,3773) | 1:34:A:VAL:HG13 | 1:37:A:LEU:HB3 | 20 | 0.16 | 0.02 | 0.16 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 20 | 0.16 | 0.02 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 20 | 0.16 | 0.01 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD13 | 1:106:A:PHE:HE1 | 20 | 0.16 | 0.01 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD12 | 1:106:A:PHE:HE1 | 20 | 0.16 | 0.01 | 0.16 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 20 | 0.15 | 0.02 | 0.16 |
| (2,3770) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 20 | 0.15 | 0.02 | 0.15 |
| (2,3770) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 20 | 0.15 | 0.02 | 0.15 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 20 | 0.15 | 0.02 | 0.15 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 20 | 0.15 | 0.02 | 0.15 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 20 | 0.15 | 0.02 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 20 | 0.15 | 0.01 | 0.15 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 20 | 0.15 | 0.01 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 20 | 0.14 | 0.01 | 0.14 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 20 | 0.13 | 0.01 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 20 | 0.13 | 0.0 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (4,274) | 1:124:A:LEU:HD22 | 1:159:A:TYR:HE1 | 19 | 1.6 | 0.43 | 1.5 |
| (4,274) | 1:124:A:LEU:HD23 | 1:159:A:TYR:HE1 | 19 | 1.6 | 0.43 | 1.5 |
| (4,274) | 1:124:A:LEU:HD21 | 1:156:A:PHE:HZ | 19 | 1.6 | 0.43 | 1.5 |
| (4,274) | 1:124:A:LEU:HD22 | 1:156:A:PHE:HZ | 19 | 1.6 | 0.43 | 1.5 |
| (4,274) | 1:124:A:LEU:HD23 | 1:156:A:PHE:HZ | 19 | 1.6 | 0.43 | 1.5 |
| (4,274) | 1:124:A:LEU:HD21 | 1:159:A:TYR:HE1 | 19 | 1.6 | 0.43 | 1.5 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 19 | 1.39 | 0.77 | 1.54 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 19 | 0.95 | 0.28 | 0.94 |
| (2,1468) | 1:22:A:ILE:HG21 | 1:10:A:PHE:HZ | 19 | 0.95 | 0.28 | 0.94 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD11 | 19 | 0.87 | 0.12 | 0.87 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 19 | 0.87 | 0.12 | 0.87 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 19 | 0.87 | 0.12 | 0.87 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 19 | 0.87 | 0.12 | 0.87 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD12 | 19 | 0.87 | 0.12 | 0.87 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 19 | 0.82 | 0.27 | 0.97 |
| (2,1549) | 1:37:A:LEU:HD12 | 1:41:A:MET:HG2 | 19 | 0.78 | 0.32 | 0.85 |
| (2,1549) | 1:37:A:LEU:HD13 | 1:41:A:MET:HG2 | 19 | 0.78 | 0.32 | 0.85 |
| (2,1549) | 1:37:A:LEU:HD11 | 1:41:A:MET:HG2 | 19 | 0.78 | 0.32 | 0.85 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD22 | 19 | 0.76 | 0.15 | 0.77 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD23 | 19 | 0.76 | 0.15 | 0.77 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD23 | 19 | 0.76 | 0.15 | 0.77 |
| (4,450) | 1:97:A:LEU:HD21 | 1:124:A:LEU:HD23 | 19 | 0.76 | 0.15 | 0.77 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD22 | 19 | 0.76 | 0.15 | 0.77 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD21 | 19 | 0.76 | 0.15 | 0.77 |
| (4,450) | 1:97:A:LEU:HD21 | 1:124:A:LEU:HD22 | 19 | 0.76 | 0.15 | 0.77 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD21 | 19 | 0.76 | 0.15 | 0.77 |
| (2,3790) | 1:34:A:VAL:HG12 | 1:50:A:MET:HE2 | 19 | 0.68 | 0.16 | 0.72 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 19 | 0.68 | 0.16 | 0.72 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 19 | 0.68 | 0.16 | 0.72 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE1 | 19 | 0.68 | 0.16 | 0.72 |
| (2,3790) | 1:34:A:VAL:HG12 | 1:50:A:MET:HE1 | 19 | 0.68 | 0.16 | 0.72 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 19 | 0.6 | 0.24 | 0.66 |
| (2,1424) | 1:56:A:ILE:HG23 | 1:65:A:PHE:HE1 | 19 | 0.6 | 0.24 | 0.66 |
| (2,1424) | 1:56:A:ILE:HG21 | 1:65:A:PHE:HE1 | 19 | 0.6 | 0.24 | 0.66 |
| (2,1807) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 19 | 0.55 | 0.24 | 0.53 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 19 | 0.55 | 0.24 | 0.53 |
| (2,1807) | 1:151:A:MET:HE3 | 1:174:A:GLU:HG2 | 19 | 0.55 | 0.24 | 0.53 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 19 | 0.55 | 0.18 | 0.51 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 19 | 0.55 | 0.18 | 0.51 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 19 | 0.55 | 0.18 | 0.51 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 19 | 0.54 | 0.14 | 0.54 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB3 | 19 | 0.54 | 0.14 | 0.54 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3837) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 19 | 0.54 | 0.33 | 0.76 |
| (2,3837) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HA | 19 | 0.54 | 0.33 | 0.76 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 19 | 0.54 | 0.33 | 0.76 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 19 | 0.47 | 0.16 | 0.48 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 19 | 0.44 | 0.05 | 0.43 |
| (2,1750) | 1:158:A:PHE:HB2 | 1:168:A:ILE:HG12 | 19 | 0.44 | 0.05 | 0.43 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 19 | 0.4 | 0.07 | 0.41 |
| (2,405) | 1:95:A:ALA:HB2 | 1:149:A:LYS:H | 19 | 0.4 | 0.07 | 0.41 |
| (2,1531) | 1:21:A:LEU:HD11 | 1:14:A:VAL:HA | 19 | 0.39 | 0.04 | 0.37 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 19 | 0.39 | 0.04 | 0.37 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 19 | 0.38 | 0.05 | 0.39 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 19 | 0.38 | 0.11 | 0.45 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 19 | 0.38 | 0.11 | 0.45 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG13 | 19 | 0.38 | 0.11 | 0.45 |
| (2,16) | 1:21:A:LEU:HD13 | 1:10:A:PHE:HE1 | 19 | 0.36 | 0.11 | 0.38 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 19 | 0.36 | 0.11 | 0.38 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 19 | 0.35 | 0.09 | 0.35 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 19 | 0.35 | 0.09 | 0.35 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 19 | 0.35 | 0.04 | 0.34 |
| (2,3718) | 1:158:A:PHE:HB2 | 1:168:A:ILE:HG12 | 19 | 0.35 | 0.04 | 0.34 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 19 | 0.34 | 0.07 | 0.35 |
| (2,2376) | 1:95:A:ALA:HB2 | 1:149:A:LYS:H | 19 | 0.34 | 0.07 | 0.35 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 19 | 0.34 | 0.08 | 0.35 |
| (2,3474) | 1:146:A:VAL:HG12 | 1:96:A:VAL:HA | 19 | 0.34 | 0.08 | 0.35 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD11 | 19 | 0.34 | 0.12 | 0.34 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 19 | 0.34 | 0.12 | 0.34 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 19 | 0.34 | 0.12 | 0.34 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 19 | 0.34 | 0.12 | 0.34 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD12 | 19 | 0.34 | 0.12 | 0.34 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 19 | 0.32 | 0.09 | 0.31 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 19 | 0.32 | 0.09 | 0.31 |
| (2,3811) | 1:15:A:LEU:HD13 | 1:74:A:ILE:HD11 | 19 | 0.32 | 0.09 | 0.31 |
| (2,3811) | 1:15:A:LEU:HD11 | 1:74:A:ILE:HD12 | 19 | 0.32 | 0.09 | 0.31 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 19 | 0.29 | 0.11 | 0.25 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 19 | 0.28 | 0.05 | 0.28 |
| (2,3490) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HA | 19 | 0.28 | 0.06 | 0.27 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 19 | 0.28 | 0.06 | 0.27 |
| (2,3490) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HA | 19 | 0.28 | 0.06 | 0.27 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 19 | 0.25 | 0.06 | 0.24 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 19 | 0.23 | 0.04 | 0.23 |
| (2,3502) | 1:21:A:LEU:HD11 | 1:14:A:VAL:HA | 19 | 0.23 | 0.04 | 0.22 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 19 | 0.23 | 0.04 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 19 | 0.22 | 0.02 | 0.22 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 19 | 0.22 | 0.05 | 0.23 |
| (2,1410) | 1:95:A:ALA:HB3 | 1:96:A:VAL:H | 19 | 0.22 | 0.05 | 0.23 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 19 | 0.21 | 0.03 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 19 | 0.21 | 0.02 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD21 | 19 | 0.21 | 0.02 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD22 | 19 | 0.21 | 0.02 | 0.21 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 19 | 0.2 | 0.02 | 0.2 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 19 | 0.18 | 0.03 | 0.18 |
| (2,3763) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD11 | 19 | 0.18 | 0.04 | 0.18 |
| (2,3763) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD12 | 19 | 0.18 | 0.04 | 0.18 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 19 | 0.18 | 0.04 | 0.18 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 19 | 0.18 | 0.04 | 0.18 |
| (2,3763) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD11 | 19 | 0.18 | 0.04 | 0.18 |
| (2,3763) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD12 | 19 | 0.18 | 0.04 | 0.18 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 19 | 0.18 | 0.03 | 0.18 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG22 | 19 | 0.18 | 0.03 | 0.18 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 19 | 0.17 | 0.04 | 0.17 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 19 | 0.16 | 0.04 | 0.15 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 19 | 0.16 | 0.06 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 19 | 0.16 | 0.06 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HB | 19 | 0.16 | 0.06 | 0.14 |
| (2,1474) | 1:110:A:LEU:HD23 | 1:110:A:LEU:H | 19 | 0.16 | 0.03 | 0.16 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 19 | 0.16 | 0.03 | 0.16 |
| (2,1474) | 1:110:A:LEU:HD21 | 1:110:A:LEU:H | 19 | 0.16 | 0.03 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG13 | 1:37:A:LEU:HB3 | 19 | 0.15 | 0.02 | 0.15 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 19 | 0.15 | 0.02 | 0.15 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 19 | 0.14 | 0.02 | 0.15 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 19 | 0.14 | 0.02 | 0.14 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 19 | 0.14 | 0.03 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 19 | 0.13 | 0.02 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 19 | 0.13 | 0.02 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 19 | 0.13 | 0.02 | 0.13 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 19 | 0.13 | 0.02 | 0.13 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 19 | 0.13 | 0.02 | 0.14 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 19 | 0.12 | 0.01 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 19 | 0.12 | 0.01 | 0.12 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 19 | 0.12 | 0.01 | 0.11 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 18 | 1.81 | 0.83 | 2.13 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG12 | 18 | 1.81 | 0.83 | 2.13 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG11 | 18 | 1.81 | 0.83 | 2.13 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 18 | 0.85 | 0.31 | 1.02 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 18 | 0.78 | 0.2 | 0.79 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 18 | 0.73 | 0.16 | 0.76 |
| (2,3524) | 1:13:A:LEU:HD11 | 1:18:A:ASN:HB2 | 18 | 0.73 | 0.16 | 0.76 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 18 | 0.66 | 0.05 | 0.66 |
| (4,6) | 1:65:A:PHE:HE1 | 1:74:A:ILE:HG23 | 18 | 0.58 | 0.15 | 0.58 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD22 | 18 | 0.58 | 0.15 | 0.58 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD21 | 18 | 0.58 | 0.15 | 0.58 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD23 | 18 | 0.58 | 0.15 | 0.58 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 18 | 0.47 | 0.11 | 0.44 |
| (2,1565) | 1:22:A:ILE:HG22 | 1:41:A:MET:HB2 | 18 | 0.47 | 0.11 | 0.44 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 18 | 0.43 | 0.11 | 0.44 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 18 | 0.42 | 0.09 | 0.43 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 18 | 0.39 | 0.07 | 0.41 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 18 | 0.38 | 0.12 | 0.41 |
| (2,1314) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 18 | 0.38 | 0.12 | 0.41 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 18 | 0.37 | 0.05 | 0.37 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 18 | 0.33 | 0.09 | 0.34 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 18 | 0.27 | 0.07 | 0.28 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 18 | 0.26 | 0.12 | 0.22 |
| (4,208) | 1:171:A:VAL:HG23 | 1:173:A:ALA:HA | 18 | 0.26 | 0.12 | 0.22 |
| (4,208) | 1:14:A:VAL:HG22 | 1:11:A:LEU:HA | 18 | 0.26 | 0.12 | 0.22 |
| (4,208) | 1:14:A:VAL:HG21 | 1:11:A:LEU:HA | 18 | 0.26 | 0.12 | 0.22 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 18 | 0.26 | 0.03 | 0.26 |
| (4,307) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 18 | 0.24 | 0.06 | 0.27 |
| (4,307) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 18 | 0.24 | 0.06 | 0.27 |
| (4,307) | 1:26:A:LEU:HD22 | 1:15:A:LEU:HA | 18 | 0.24 | 0.06 | 0.27 |
| (4,307) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 18 | 0.24 | 0.06 | 0.27 |
| (4,307) | 1:38:A:LEU:HD12 | 1:50:A:MET:HA | 18 | 0.24 | 0.06 | 0.27 |
| (4,307) | 1:26:A:LEU:HD21 | 1:15:A:LEU:HA | 18 | 0.24 | 0.06 | 0.27 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 18 | 0.24 | 0.06 | 0.26 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 18 | 0.24 | 0.04 | 0.24 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 18 | 0.24 | 0.04 | 0.24 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG22 | 18 | 0.24 | 0.04 | 0.24 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 18 | 0.23 | 0.09 | 0.24 |
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 18 | 0.23 | 0.09 | 0.24 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG11 | 18 | 0.22 | 0.04 | 0.24 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 18 | 0.22 | 0.04 | 0.24 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 18 | 0.21 | 0.03 | 0.22 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 18 | 0.2 | 0.05 | 0.22 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 18 | 0.2 | 0.05 | 0.19 |
| (2,3266) | 1:53:A:LEU:HD11 | 1:67:A:PHE:HE1 | 18 | 0.2 | 0.05 | 0.19 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 18 | 0.19 | 0.03 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 18 | 0.18 | 0.03 | 0.2 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 18 | 0.17 | 0.03 | 0.17 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 18 | 0.17 | 0.03 | 0.17 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD23 | 18 | 0.17 | 0.03 | 0.17 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 18 | 0.17 | 0.03 | 0.16 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 18 | 0.17 | 0.02 | 0.16 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 18 | 0.17 | 0.02 | 0.16 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB3 | 18 | 0.17 | 0.02 | 0.16 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 18 | 0.16 | 0.02 | 0.16 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 18 | 0.16 | 0.02 | 0.17 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 18 | 0.15 | 0.02 | 0.15 |
| (2,85) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 18 | 0.14 | 0.02 | 0.14 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 18 | 0.14 | 0.02 | 0.14 |
| (2,3802) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 18 | 0.14 | 0.02 | 0.14 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 18 | 0.14 | 0.02 | 0.14 |
| (2,3802) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 18 | 0.14 | 0.02 | 0.14 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 18 | 0.13 | 0.01 | 0.13 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 18 | 0.13 | 0.02 | 0.13 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 18 | 0.12 | 0.01 | 0.13 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 18 | 0.12 | 0.01 | 0.12 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 17 | 0.77 | 0.35 | 0.81 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 17 | 0.77 | 0.35 | 0.81 |
| (4,353) | 1:84:A:VAL:HB | 1:87:A:GLY:HA2 | 17 | 0.77 | 0.35 | 0.81 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 17 | 0.77 | 0.12 | 0.8 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 17 | 0.7 | 0.21 | 0.69 |
| (4,95) | 1:51:A:GLU:H | 1:58:A:GLU:HG3 | 17 | 0.7 | 0.21 | 0.69 |
| (4,332) | 1:37:A:LEU:HD12 | 1:41:A:MET:HB2 | 17 | 0.65 | 0.1 | 0.63 |
| (4,332) | 1:37:A:LEU:HD13 | 1:41:A:MET:HB2 | 17 | 0.65 | 0.1 | 0.63 |
| (4,332) | 1:37:A:LEU:HD11 | 1:41:A:MET:HB2 | 17 | 0.65 | 0.1 | 0.63 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 17 | 0.55 | 0.23 | 0.59 |
| (2,1601) | 1:41:A:MET:HE2 | 1:10:A:PHE:HB3 | 17 | 0.55 | 0.23 | 0.59 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 17 | 0.47 | 0.17 | 0.44 |
| (2,3772) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 17 | 0.44 | 0.21 | 0.44 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 17 | 0.44 | 0.21 | 0.44 |
| (2,3772) | 1:151:A:MET:HE3 | 1:174:A:GLU:HG2 | 17 | 0.44 | 0.21 | 0.44 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 17 | 0.44 | 0.38 | 0.3 |
| (2,815) | 1:102:A:ALA:H | 1:101:A:THR:HG23 | 17 | 0.44 | 0.38 | 0.3 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 17 | 0.43 | 0.1 | 0.47 |
| (2,3391) | 1:56:A:ILE:HG23 | 1:65:A:PHE:HD1 | 17 | 0.43 | 0.1 | 0.47 |
| (2,3391) | 1:56:A:ILE:HG21 | 1:65:A:PHE:HD1 | 17 | 0.43 | 0.1 | 0.47 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 17 | 0.41 | 0.2 | 0.35 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 17 | 0.38 | 0.05 | 0.37 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG21 | 17 | 0.38 | 0.05 | 0.37 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 17 | 0.37 | 0.02 | 0.37 |
| (2,521) | 1:129:A:THR:HG23 | 1:129:A:THR:H | 17 | 0.37 | 0.02 | 0.37 |
| (2,521) | 1:129:A:THR:HG22 | 1:129:A:THR:H | 17 | 0.37 | 0.02 | 0.37 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 17 | 0.31 | 0.17 | 0.28 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 17 | 0.31 | 0.17 | 0.28 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 17 | 0.31 | 0.17 | 0.28 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 17 | 0.28 | 0.14 | 0.27 |
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 17 | 0.28 | 0.14 | 0.27 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 17 | 0.25 | 0.08 | 0.22 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD13 | 17 | 0.24 | 0.06 | 0.23 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD11 | 17 | 0.24 | 0.06 | 0.23 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD12 | 17 | 0.24 | 0.06 | 0.23 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 17 | 0.22 | 0.05 | 0.22 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 17 | 0.2 | 0.05 | 0.2 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG23 | 17 | 0.2 | 0.05 | 0.2 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 17 | 0.2 | 0.04 | 0.21 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 17 | 0.19 | 0.03 | 0.19 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 17 | 0.18 | 0.05 | 0.17 |
| (4,290) | 1:53:A:LEU:HD22 | 1:56:A:ILE:H | 17 | 0.18 | 0.05 | 0.17 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 17 | 0.18 | 0.05 | 0.18 |
| (4,442) | 1:178:A:VAL:HG21 | 1:144:A:LEU:HG | 17 | 0.18 | 0.05 | 0.18 |
| (4,442) | 1:178:A:VAL:HG22 | 1:176:A:ILE:HB | 17 | 0.18 | 0.05 | 0.18 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 17 | 0.17 | 0.03 | 0.18 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 17 | 0.17 | 0.02 | 0.17 |
| (2,3382) | 1:53:A:LEU:HD11 | 1:67:A:PHE:HZ | 17 | 0.17 | 0.02 | 0.17 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 17 | 0.16 | 0.03 | 0.15 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 17 | 0.16 | 0.03 | 0.15 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG11 | 17 | 0.16 | 0.02 | 0.16 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 17 | 0.16 | 0.02 | 0.16 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 17 | 0.15 | 0.03 | 0.15 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 17 | 0.15 | 0.03 | 0.15 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG22 | 17 | 0.15 | 0.03 | 0.15 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 17 | 0.13 | 0.02 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG23 | 1:57:A:VAL:H | 17 | 0.13 | 0.02 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG21 | 1:57:A:VAL:H | 17 | 0.13 | 0.02 | 0.14 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 17 | 0.13 | 0.02 | 0.13 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 17 | 0.13 | 0.02 | 0.13 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB3 | 17 | 0.13 | 0.02 | 0.13 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 17 | 0.12 | 0.01 | 0.12 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 17 | 0.12 | 0.01 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 17 | 0.11 | 0.01 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1291) | 1:84:A:VAL:HG13 | 1:84:A:VAL:H | 16 | 0.98 | 0.29 | 0.94 |
| (2,1291) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 16 | 0.98 | 0.29 | 0.94 |
| (2,1291) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 16 | 0.98 | 0.29 | 0.94 |
| (2,3416) | 1:143:A:VAL:HG13 | 1:143:A:VAL:H | 16 | 0.71 | 0.05 | 0.71 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 16 | 0.71 | 0.05 | 0.71 |
| (2,3416) | 1:143:A:VAL:HG11 | 1:143:A:VAL:H | 16 | 0.71 | 0.05 | 0.71 |
| (2,3265) | 1:84:A:VAL:HG13 | 1:84:A:VAL:H | 16 | 0.71 | 0.29 | 0.66 |
| (2,3265) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 16 | 0.71 | 0.29 | 0.66 |
| (2,3265) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 16 | 0.71 | 0.29 | 0.66 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 16 | 0.67 | 0.1 | 0.66 |
| (2,3784) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 16 | 0.67 | 0.1 | 0.66 |
| (2,3784) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE3 | 16 | 0.67 | 0.1 | 0.66 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE3 | 16 | 0.67 | 0.1 | 0.66 |
| (2,3784) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE1 | 16 | 0.67 | 0.1 | 0.66 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 16 | 0.61 | 0.1 | 0.6 |
| (2,1823) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 16 | 0.61 | 0.1 | 0.6 |
| (2,1823) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE3 | 16 | 0.61 | 0.1 | 0.6 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE3 | 16 | 0.61 | 0.1 | 0.6 |
| (2,1823) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE1 | 16 | 0.61 | 0.1 | 0.6 |
| (2,3570) | 1:4:A:MET:HE3 | 1:52:A:GLU:HA | 16 | 0.5 | 0.21 | 0.48 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 16 | 0.5 | 0.21 | 0.48 |
| (2,3570) | 1:4:A:MET:HE2 | 1:52:A:GLU:HA | 16 | 0.5 | 0.21 | 0.48 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 16 | 0.4 | 0.13 | 0.4 |
| (2,187) | 1:26:A:LEU:HD22 | 1:26:A:LEU:H | 16 | 0.4 | 0.13 | 0.4 |
| (2,187) | 1:26:A:LEU:HD23 | 1:26:A:LEU:H | 16 | 0.4 | 0.13 | 0.4 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 16 | 0.34 | 0.08 | 0.34 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 16 | 0.32 | 0.16 | 0.24 |
| (2,1388) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 16 | 0.32 | 0.16 | 0.24 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 16 | 0.23 | 0.07 | 0.22 |
| (2,1509) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 16 | 0.23 | 0.07 | 0.22 |
| (2,1509) | 1:151:A:MET:HE3 | 1:171:A:VAL:HA | 16 | 0.23 | 0.07 | 0.22 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 16 | 0.21 | 0.11 | 0.16 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 16 | 0.2 | 0.02 | 0.2 |
| (2,594) | 1:43:A:ALA:HB1 | 1:44:A:LYS:H | 16 | 0.2 | 0.02 | 0.2 |
| (2,594) | 1:43:A:ALA:HB3 | 1:44:A:LYS:H | 16 | 0.2 | 0.02 | 0.2 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 16 | 0.17 | 0.04 | 0.17 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 16 | 0.16 | 0.02 | 0.16 |
| (2,2367) | 1:48:A:ILE:HG23 | 1:48:A:ILE:H | 16 | 0.16 | 0.02 | 0.16 |
| (2,2367) | 1:48:A:ILE:HG22 | 1:48:A:ILE:H | 16 | 0.16 | 0.02 | 0.16 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 16 | 0.16 | 0.05 | 0.15 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG21 | 16 | 0.16 | 0.05 | 0.15 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 16 | 0.15 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 16 | 0.14 | 0.04 | 0.11 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 16 | 0.13 | 0.03 | 0.11 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 16 | 0.12 | 0.01 | 0.12 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 16 | 0.12 | 0.01 | 0.12 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 16 | 0.12 | 0.01 | 0.12 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 16 | 0.12 | 0.01 | 0.12 |
| (4,41) | 1:5:A:VAL:HG22 | 1:5:A:VAL:H | 16 | 0.12 | 0.01 | 0.12 |
| (4,41) | 1:5:A:VAL:HG23 | 1:5:A:VAL:H | 16 | 0.12 | 0.01 | 0.12 |
| (4,41) | 1:5:A:VAL:HG21 | 1:5:A:VAL:H | 16 | 0.12 | 0.01 | 0.12 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 16 | 0.12 | 0.01 | 0.12 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 16 | 0.12 | 0.01 | 0.12 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 15 | 0.76 | 0.43 | 1.01 |
| (4,440) | 1:15:A:LEU:HD23 | 1:74:A:ILE:HB | 15 | 0.76 | 0.43 | 1.01 |
| (4,440) | 1:15:A:LEU:HD23 | 1:13:A:LEU:HB2 | 15 | 0.76 | 0.43 | 1.01 |
| (4,440) | 1:15:A:LEU:HD22 | 1:13:A:LEU:HB2 | 15 | 0.76 | 0.43 | 1.01 |
| (4,320) | 1:151:A:MET:HE2 | 1:147:A:ASP:HB2 | 15 | 0.75 | 0.4 | 0.71 |
| (4,320) | 1:151:A:MET:HE3 | 1:158:A:PHE:HB3 | 15 | 0.75 | 0.4 | 0.71 |
| (4,320) | 1:151:A:MET:HE1 | 1:147:A:ASP:HB2 | 15 | 0.75 | 0.4 | 0.71 |
| (4,320) | 1:151:A:MET:HE3 | 1:147:A:ASP:HB2 | 15 | 0.75 | 0.4 | 0.71 |
| (4,320) | 1:151:A:MET:HE2 | 1:158:A:PHE:HB2 | 15 | 0.75 | 0.4 | 0.71 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 15 | 0.57 | 0.16 | 0.59 |
| (2,1482) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 15 | 0.57 | 0.16 | 0.59 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 15 | 0.45 | 0.13 | 0.48 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HG3 | 15 | 0.45 | 0.13 | 0.48 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 15 | 0.43 | 0.21 | 0.38 |
| (2,1871) | 1:97:A:LEU:HD22 | 1:151:A:MET:HG3 | 15 | 0.43 | 0.21 | 0.38 |
| (2,1871) | 1:97:A:LEU:HD21 | 1:151:A:MET:HG3 | 15 | 0.43 | 0.21 | 0.38 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 15 | 0.41 | 0.21 | 0.3 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 15 | 0.35 | 0.18 | 0.28 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 15 | 0.31 | 0.06 | 0.31 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 15 | 0.31 | 0.09 | 0.31 |
| (2,3467) | 1:11:A:LEU:HD12 | 1:38:A:LEU:HA | 15 | 0.31 | 0.09 | 0.31 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 15 | 0.26 | 0.1 | 0.26 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 15 | 0.23 | 0.08 | 0.21 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 15 | 0.23 | 0.05 | 0.21 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 15 | 0.23 | 0.05 | 0.22 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 15 | 0.22 | 0.04 | 0.22 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 15 | 0.2 | 0.03 | 0.2 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 15 | 0.2 | 0.04 | 0.21 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 15 | 0.19 | 0.04 | 0.2 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 15 | 0.16 | 0.03 | 0.16 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 15 | 0.15 | 0.03 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 15 | 0.14 | 0.02 | 0.13 |
| (4,69) | 1:37:A:LEU:H | 1:53:A:LEU:HD11 | 15 | 0.14 | 0.02 | 0.13 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 15 | 0.13 | 0.02 | 0.13 |
| (2,2566) | 1:43:A:ALA:HB1 | 1:44:A:LYS:H | 15 | 0.13 | 0.02 | 0.13 |
| (2,2566) | 1:43:A:ALA:HB3 | 1:44:A:LYS:H | 15 | 0.13 | 0.02 | 0.13 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 15 | 0.13 | 0.01 | 0.13 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 15 | 0.13 | 0.01 | 0.13 |
| (2,1492) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 14 | 0.84 | 0.34 | 0.82 |
| (2,1492) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 14 | 0.84 | 0.34 | 0.82 |
| (2,1492) | 1:167:A:LEU:HD21 | 1:123:A:HIS:HA | 14 | 0.84 | 0.34 | 0.82 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 14 | 0.84 | 0.25 | 0.92 |
| (2,21) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 14 | 0.84 | 0.25 | 0.92 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD12 | 14 | 0.84 | 0.25 | 0.92 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 14 | 0.49 | 0.14 | 0.52 |
| (4,283) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 14 | 0.49 | 0.14 | 0.52 |
| (4,311) | 1:143:A:VAL:HG13 | 1:178:A:VAL:HA | 14 | 0.38 | 0.22 | 0.36 |
| (4,311) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 14 | 0.38 | 0.22 | 0.36 |
| (4,311) | 1:143:A:VAL:HG11 | 1:178:A:VAL:HA | 14 | 0.38 | 0.22 | 0.36 |
| (4,311) | 1:143:A:VAL:HG12 | 1:178:A:VAL:HA | 14 | 0.38 | 0.22 | 0.36 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 14 | 0.38 | 0.15 | 0.4 |
| (2,3390) | 1:56:A:ILE:HG23 | 1:65:A:PHE:HE1 | 14 | 0.38 | 0.15 | 0.4 |
| (2,3390) | 1:56:A:ILE:HG21 | 1:65:A:PHE:HE1 | 14 | 0.38 | 0.15 | 0.4 |
| (4,328) | 1:122:A:VAL:HG13 | 1:113:A:GLY:HA2 | 14 | 0.37 | 0.18 | 0.32 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 14 | 0.37 | 0.18 | 0.32 |
| (4,328) | 1:122:A:VAL:HG12 | 1:113:A:GLY:HA2 | 14 | 0.37 | 0.18 | 0.32 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 14 | 0.22 | 0.05 | 0.21 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 14 | 0.21 | 0.08 | 0.18 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD23 | 14 | 0.21 | 0.08 | 0.18 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD22 | 14 | 0.21 | 0.08 | 0.18 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 14 | 0.18 | 0.04 | 0.17 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 14 | 0.15 | 0.02 | 0.14 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 14 | 0.15 | 0.02 | 0.14 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 14 | 0.14 | 0.03 | 0.13 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 14 | 0.14 | 0.03 | 0.13 |
| (2,3473) | 1:146:A:VAL:HG23 | 1:96:A:VAL:HA | 14 | 0.14 | 0.03 | 0.13 |
| (2,3473) | 1:146:A:VAL:HG22 | 1:96:A:VAL:HA | 14 | 0.14 | 0.03 | 0.13 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 14 | 0.14 | 0.03 | 0.14 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 14 | 0.13 | 0.02 | 0.13 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 14 | 0.12 | 0.02 | 0.12 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 14 | 0.12 | 0.02 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HB2 | 14 | 0.12 | 0.01 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 14 | 0.12 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3519) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 14 | 0.12 | 0.01 | 0.12 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 13 | 1.43 | 0.67 | 1.4 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 13 | 1.11 | 0.18 | 1.12 |
| (4,292) | 1:122:A:VAL:HG23 | 1:118:A:SER:H | 13 | 0.91 | 0.45 | 0.87 |
| (4,292) | 1:122:A:VAL:HG22 | 1:118:A:SER:H | 13 | 0.91 | 0.45 | 0.87 |
| (4,292) | 1:122:A:VAL:HG21 | 1:118:A:SER:H | 13 | 0.91 | 0.45 | 0.87 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 13 | 0.7 | 0.04 | 0.72 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 13 | 0.6 | 0.34 | 0.58 |
| (4,350) | 1:42:A:LYS:HE3 | 1:44:A:LYS:HG2 | 13 | 0.6 | 0.34 | 0.58 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG2 | 13 | 0.6 | 0.34 | 0.58 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 13 | 0.47 | 0.17 | 0.49 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE2 | 13 | 0.38 | 0.11 | 0.42 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 13 | 0.38 | 0.11 | 0.42 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 13 | 0.35 | 0.04 | 0.34 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 13 | 0.34 | 0.11 | 0.35 |
| (2,2521) | 1:105:A:ASN:H | 1:102:A:ALA:HB3 | 13 | 0.34 | 0.11 | 0.35 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB3 | 13 | 0.33 | 0.14 | 0.29 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB2 | 13 | 0.33 | 0.14 | 0.29 |
| (2,3484) | 1:124:A:LEU:HD12 | 1:167:A:LEU:HA | 13 | 0.29 | 0.07 | 0.29 |
| (2,3484) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 13 | 0.29 | 0.07 | 0.29 |
| (2,3484) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 13 | 0.29 | 0.07 | 0.29 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 13 | 0.28 | 0.11 | 0.3 |
| (2,1710) | 1:26:A:LEU:HD21 | 1:15:A:LEU:HA | 13 | 0.28 | 0.11 | 0.3 |
| (2,1710) | 1:26:A:LEU:HD22 | 1:15:A:LEU:HA | 13 | 0.28 | 0.11 | 0.3 |
| (2,1514) | 1:124:A:LEU:HD12 | 1:167:A:LEU:HA | 13 | 0.27 | 0.07 | 0.27 |
| (2,1514) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 13 | 0.27 | 0.07 | 0.27 |
| (2,1514) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 13 | 0.27 | 0.07 | 0.27 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 13 | 0.2 | 0.04 | 0.21 |
| (2,3479) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 13 | 0.19 | 0.07 | 0.19 |
| (2,3479) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 13 | 0.19 | 0.07 | 0.19 |
| (2,3479) | 1:151:A:MET:HE3 | 1:171:A:VAL:HA | 13 | 0.19 | 0.07 | 0.19 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 13 | 0.15 | 0.02 | 0.15 |
| (2,3575) | 1:50:A:MET:HE1 | 1:50:A:MET:HG3 | 13 | 0.15 | 0.03 | 0.14 |
| (2,3575) | 1:50:A:MET:HE2 | 1:50:A:MET:HG3 | 13 | 0.15 | 0.03 | 0.14 |
| (2,3575) | 1:50:A:MET:HE3 | 1:50:A:MET:HG3 | 13 | 0.15 | 0.03 | 0.14 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 13 | 0.15 | 0.02 | 0.14 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 13 | 0.13 | 0.04 | 0.12 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 13 | 0.13 | 0.02 | 0.13 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 13 | 0.13 | 0.06 | 0.11 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 12 | 0.85 | 0.23 | 0.77 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 12 | 0.66 | 0.23 | 0.65 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 12 | 0.54 | 0.11 | 0.58 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1974) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 12 | 0.54 | 0.11 | 0.58 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD12 | 12 | 0.54 | 0.11 | 0.58 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 12 | 0.51 | 0.26 | 0.5 |
| (2,1534) | 1:151:A:MET:HE2 | 1:151:A:MET:HA | 12 | 0.44 | 0.1 | 0.45 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 12 | 0.44 | 0.1 | 0.45 |
| (2,1534) | 1:151:A:MET:HE3 | 1:151:A:MET:HA | 12 | 0.44 | 0.1 | 0.45 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 12 | 0.43 | 0.26 | 0.34 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 12 | 0.37 | 0.14 | 0.42 |
| (2,1599) | 1:4:A:MET:HE3 | 1:52:A:GLU:HA | 12 | 0.26 | 0.17 | 0.2 |
| (2,1599) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 12 | 0.26 | 0.17 | 0.2 |
| (2,1599) | 1:4:A:MET:HE2 | 1:52:A:GLU:HA | 12 | 0.26 | 0.17 | 0.2 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 12 | 0.23 | 0.08 | 0.22 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB3 | 12 | 0.23 | 0.08 | 0.22 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 12 | 0.22 | 0.09 | 0.25 |
| (2,3371) | 1:20:A:ALA:HB2 | 1:18:A:ASN:HD21 | 12 | 0.22 | 0.09 | 0.25 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 12 | 0.22 | 0.11 | 0.16 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 12 | 0.22 | 0.05 | 0.23 |
| (2,3434) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HE1 | 12 | 0.22 | 0.09 | 0.22 |
| (2,3434) | 1:15:A:LEU:HD12 | 1:65:A:PHE:HE1 | 12 | 0.22 | 0.09 | 0.22 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 12 | 0.22 | 0.04 | 0.22 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 12 | 0.19 | 0.03 | 0.21 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 12 | 0.17 | 0.04 | 0.16 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 12 | 0.17 | 0.04 | 0.16 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 12 | 0.15 | 0.02 | 0.15 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 12 | 0.13 | 0.02 | 0.13 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 12 | 0.13 | 0.02 | 0.13 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 12 | 0.12 | 0.02 | 0.12 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 11 | 0.87 | 0.48 | 0.85 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 11 | 0.68 | 0.05 | 0.66 |
| (2,1875) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 11 | 0.68 | 0.05 | 0.66 |
| (2,3527) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 11 | 0.62 | 0.29 | 0.52 |
| (2,3527) | 1:84:A:VAL:HG21 | 1:85:A:ASP:HB2 | 11 | 0.62 | 0.29 | 0.52 |
| (2,3527) | 1:84:A:VAL:HG23 | 1:85:A:ASP:HB2 | 11 | 0.62 | 0.29 | 0.52 |
| (2,1490) | 1:167:A:LEU:HD12 | 1:166:A:TRP:HA | 11 | 0.57 | 0.19 | 0.53 |
| (2,1490) | 1:167:A:LEU:HD13 | 1:166:A:TRP:HA | 11 | 0.57 | 0.19 | 0.53 |
| (2,1490) | 1:167:A:LEU:HD11 | 1:166:A:TRP:HA | 11 | 0.57 | 0.19 | 0.53 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 11 | 0.49 | 0.28 | 0.43 |
| (2,3514) | 1:143:A:VAL:HG12 | 1:132:A:ARG:HA | 11 | 0.43 | 0.15 | 0.46 |
| (2,3514) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 11 | 0.43 | 0.15 | 0.46 |
| (2,3514) | 1:143:A:VAL:HG13 | 1:132:A:ARG:HA | 11 | 0.43 | 0.15 | 0.46 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 11 | 0.42 | 0.4 | 0.24 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB2 | 11 | 0.42 | 0.4 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 11 | 0.25 | 0.07 | 0.25 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 11 | 0.25 | 0.07 | 0.24 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 11 | 0.23 | 0.08 | 0.22 |
| (2,2148) | 1:26:A:LEU:HD23 | 1:26:A:LEU:H | 11 | 0.23 | 0.08 | 0.22 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 11 | 0.21 | 0.09 | 0.17 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 11 | 0.17 | 0.04 | 0.17 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 11 | 0.16 | 0.06 | 0.16 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 11 | 0.15 | 0.03 | 0.14 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 11 | 0.14 | 0.02 | 0.14 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 11 | 0.13 | 0.02 | 0.14 |
| (2,1540) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HA | 11 | 0.13 | 0.02 | 0.14 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 11 | 0.12 | 0.01 | 0.12 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 10 | 0.64 | 0.24 | 0.64 |
| (4,458) | 1:50:A:MET:HE2 | 1:50:A:MET:HA | 10 | 0.64 | 0.24 | 0.64 |
| (4,458) | 1:50:A:MET:HE2 | 1:51:A:GLU:HA | 10 | 0.64 | 0.24 | 0.64 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 10 | 0.48 | 0.29 | 0.45 |
| (2,1377) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 10 | 0.45 | 0.13 | 0.42 |
| (2,1377) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 10 | 0.45 | 0.13 | 0.42 |
| (2,1377) | 1:4:A:MET:HE2 | 1:55:A:HIS:HD2 | 10 | 0.45 | 0.13 | 0.42 |
| (2,3346) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 10 | 0.43 | 0.14 | 0.41 |
| (2,3346) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 10 | 0.43 | 0.14 | 0.41 |
| (2,3346) | 1:4:A:MET:HE2 | 1:55:A:HIS:HD2 | 10 | 0.43 | 0.14 | 0.41 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 10 | 0.41 | 0.18 | 0.36 |
| (2,1378) | 1:50:A:MET:HE2 | 1:67:A:PHE:HZ | 10 | 0.41 | 0.18 | 0.36 |
| (2,1378) | 1:50:A:MET:HE1 | 1:67:A:PHE:HZ | 10 | 0.41 | 0.18 | 0.36 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 10 | 0.36 | 0.12 | 0.38 |
| (2,1541) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 10 | 0.36 | 0.11 | 0.36 |
| (2,1541) | 1:143:A:VAL:HG13 | 1:132:A:ARG:HA | 10 | 0.36 | 0.11 | 0.36 |
| (2,1541) | 1:143:A:VAL:HG12 | 1:132:A:ARG:HA | 10 | 0.36 | 0.11 | 0.36 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 10 | 0.33 | 0.1 | 0.34 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 10 | 0.32 | 0.09 | 0.34 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 10 | 0.32 | 0.07 | 0.33 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 10 | 0.3 | 0.11 | 0.28 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 10 | 0.25 | 0.13 | 0.18 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 10 | 0.25 | 0.13 | 0.18 |
| (2,3288) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 10 | 0.18 | 0.07 | 0.16 |
| (2,3288) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 10 | 0.18 | 0.07 | 0.16 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 10 | 0.18 | 0.02 | 0.18 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 10 | 0.17 | 0.04 | 0.16 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 10 | 0.14 | 0.04 | 0.14 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 10 | 0.14 | 0.02 | 0.14 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD13 | 10 | 0.14 | 0.02 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3812) | 1:56:A:ILE:HG21 | 1:11:A:LEU:HD11 | 10 | 0.14 | 0.02 | 0.14 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 10 | 0.14 | 0.03 | 0.13 |
| (2,3820) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HD11 | 10 | 0.14 | 0.03 | 0.12 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 10 | 0.14 | 0.03 | 0.12 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 10 | 0.14 | 0.03 | 0.12 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 10 | 0.13 | 0.03 | 0.12 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 10 | 0.13 | 0.03 | 0.12 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 10 | 0.12 | 0.02 | 0.12 |
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 10 | 0.12 | 0.04 | 0.12 |
| (2,3376) | 1:95:A:ALA:HB3 | 1:96:A:VAL:H | 10 | 0.12 | 0.04 | 0.12 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 10 | 0.12 | 0.02 | 0.12 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 10 | 0.12 | 0.01 | 0.12 |
| (2,1440) | 1:37:A:LEU:HD12 | 1:37:A:LEU:H | 10 | 0.11 | 0.01 | 0.11 |
| (2,1440) | 1:37:A:LEU:HD11 | 1:37:A:LEU:H | 10 | 0.11 | 0.01 | 0.11 |
| (2,1440) | 1:37:A:LEU:HD13 | 1:37:A:LEU:H | 10 | 0.11 | 0.01 | 0.11 |
| (4,415) | 1:19:A:PRO:HB3 | 1:36:A:GLU:HG2 | 9 | 1.08 | 0.46 | 1.16 |
| (4,415) | 1:19:A:PRO:HB2 | 1:33:A:PRO:HG2 | 9 | 1.08 | 0.46 | 1.16 |
| (4,415) | 1:19:A:PRO:HB2 | 1:36:A:GLU:HG2 | 9 | 1.08 | 0.46 | 1.16 |
| (4,415) | 1:19:A:PRO:HB3 | 1:33:A:PRO:HG2 | 9 | 1.08 | 0.46 | 1.16 |
| (2,3847) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 9 | 0.83 | 0.22 | 0.92 |
| (2,3847) | 1:41:A:MET:HE1 | 1:46:A:HIS:HA | 9 | 0.83 | 0.22 | 0.92 |
| (2,3847) | 1:41:A:MET:HE3 | 1:46:A:HIS:HA | 9 | 0.83 | 0.22 | 0.92 |
| (4,166) | 1:171:A:VAL:H | 1:168:A:ILE:HG13 | 9 | 0.52 | 0.28 | 0.65 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD12 | 9 | 0.52 | 0.28 | 0.65 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD13 | 9 | 0.52 | 0.28 | 0.65 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD11 | 9 | 0.52 | 0.28 | 0.65 |
| (2,3600) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 9 | 0.41 | 0.09 | 0.36 |
| (2,3600) | 1:42:A:LYS:HE3 | 1:39:A:ALA:HA | 9 | 0.41 | 0.09 | 0.36 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 9 | 0.37 | 0.21 | 0.27 |
| (2,3428) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 9 | 0.35 | 0.13 | 0.34 |
| (2,3428) | 1:108:A:LEU:HD12 | 2:201:A:NAD:H2A | 9 | 0.35 | 0.13 | 0.34 |
| (2,3428) | 1:108:A:LEU:HD13 | 2:201:A:NAD:H2A | 9 | 0.35 | 0.13 | 0.34 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 9 | 0.34 | 0.16 | 0.35 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 9 | 0.31 | 0.07 | 0.31 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE1 | 9 | 0.31 | 0.07 | 0.31 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE2 | 9 | 0.31 | 0.07 | 0.31 |
| (4,325) | 1:7:A:VAL:HG13 | 1:10:A:PHE:HB3 | 9 | 0.28 | 0.15 | 0.2 |
| (4,325) | 1:7:A:VAL:HG11 | 1:10:A:PHE:HB3 | 9 | 0.28 | 0.15 | 0.2 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 9 | 0.27 | 0.06 | 0.27 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 9 | 0.27 | 0.08 | 0.29 |
| (4,379) | 1:50:A:MET:HA | 1:39:A:ALA:HB3 | 9 | 0.26 | 0.13 | 0.21 |
| (4,379) | 1:50:A:MET:HA | 1:35:A:LYS:HG2 | 9 | 0.26 | 0.13 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3409) | 1:84:A:VAL:HG13 | 1:85:A:ASP:H | 9 | 0.26 | 0.12 | 0.24 |
| (2,3409) | 1:84:A:VAL:HG11 | 1:85:A:ASP:H | 9 | 0.26 | 0.12 | 0.24 |
| (2,3409) | 1:84:A:VAL:HG12 | 1:85:A:ASP:H | 9 | 0.26 | 0.12 | 0.24 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 9 | 0.25 | 0.05 | 0.24 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD11 | 9 | 0.25 | 0.05 | 0.24 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 9 | 0.23 | 0.07 | 0.23 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE1 | 9 | 0.23 | 0.07 | 0.23 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE2 | 9 | 0.23 | 0.07 | 0.23 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 9 | 0.22 | 0.07 | 0.22 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB3 | 9 | 0.22 | 0.07 | 0.22 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 9 | 0.22 | 0.05 | 0.22 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD11 | 9 | 0.22 | 0.05 | 0.22 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 9 | 0.2 | 0.06 | 0.2 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 9 | 0.18 | 0.03 | 0.18 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 9 | 0.17 | 0.06 | 0.22 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB3 | 9 | 0.17 | 0.06 | 0.22 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 9 | 0.15 | 0.07 | 0.14 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 9 | 0.15 | 0.02 | 0.15 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 9 | 0.15 | 0.04 | 0.14 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 9 | 0.14 | 0.03 | 0.14 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 9 | 0.13 | 0.03 | 0.12 |
| (4,198) | 1:176:A:ILE:HD13 | 1:106:A:PHE:HE1 | 9 | 0.13 | 0.03 | 0.12 |
| (4,198) | 1:176:A:ILE:HD11 | 1:106:A:PHE:HE1 | 9 | 0.13 | 0.03 | 0.12 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 9 | 0.12 | 0.02 | 0.11 |
| (2,3362) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 9 | 0.12 | 0.01 | 0.12 |
| (2,3362) | 1:39:A:ALA:HB3 | 1:40:A:LYS:H | 9 | 0.12 | 0.01 | 0.12 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 9 | 0.12 | 0.01 | 0.11 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 9 | 0.11 | 0.01 | 0.11 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 8 | 1.16 | 0.54 | 1.26 |
| (2,3466) | 1:97:A:LEU:HD21 | 1:166:A:TRP:HB2 | 8 | 0.59 | 0.11 | 0.64 |
| (2,3466) | 1:97:A:LEU:HD22 | 1:166:A:TRP:HB2 | 8 | 0.59 | 0.11 | 0.64 |
| (2,1884) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 8 | 0.59 | 0.17 | 0.63 |
| (2,1884) | 1:41:A:MET:HE1 | 1:46:A:HIS:HA | 8 | 0.59 | 0.17 | 0.63 |
| (2,1884) | 1:41:A:MET:HE3 | 1:46:A:HIS:HA | 8 | 0.59 | 0.17 | 0.63 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 8 | 0.44 | 0.1 | 0.46 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 8 | 0.42 | 0.01 | 0.42 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 8 | 0.41 | 0.01 | 0.4 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 8 | 0.39 | 0.22 | 0.33 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 8 | 0.37 | 0.03 | 0.38 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD21 | 8 | 0.36 | 0.12 | 0.37 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD23 | 8 | 0.36 | 0.12 | 0.37 |
| (2,3832) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 8 | 0.36 | 0.13 | 0.38 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3832) | 1:97:A:LEU:HD22 | 1:151:A:MET:HG3 | 8 | 0.36 | 0.13 | 0.38 |
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 8 | 0.32 | 0.2 | 0.29 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 8 | 0.28 | 0.07 | 0.3 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 8 | 0.21 | 0.03 | 0.22 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 8 | 0.21 | 0.09 | 0.2 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD11 | 8 | 0.21 | 0.09 | 0.2 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD13 | 8 | 0.21 | 0.09 | 0.2 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 8 | 0.17 | 0.09 | 0.12 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 8 | 0.17 | 0.02 | 0.18 |
| (2,3518) | 1:128:A:ILE:HD12 | 1:128:A:ILE:HA | 8 | 0.15 | 0.03 | 0.15 |
| (2,3518) | 1:128:A:ILE:HD13 | 1:128:A:ILE:HA | 8 | 0.15 | 0.03 | 0.15 |
| (2,3518) | 1:128:A:ILE:HD11 | 1:128:A:ILE:HA | 8 | 0.15 | 0.03 | 0.15 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 8 | 0.15 | 0.03 | 0.15 |
| (2,2210) | 1:48:A:ILE:HD13 | 1:53:A:LEU:H | 8 | 0.14 | 0.04 | 0.13 |
| (2,2210) | 1:48:A:ILE:HD12 | 1:53:A:LEU:H | 8 | 0.14 | 0.04 | 0.13 |
| (2,2210) | 1:48:A:ILE:HD11 | 1:53:A:LEU:H | 8 | 0.14 | 0.04 | 0.13 |
| (4,61) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 8 | 0.14 | 0.02 | 0.13 |
| (4,61) | 1:37:A:LEU:H | 1:38:A:LEU:HD23 | 8 | 0.14 | 0.02 | 0.13 |
| (2,1723) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 8 | 0.12 | 0.02 | 0.12 |
| (2,1723) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 8 | 0.12 | 0.02 | 0.12 |
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 8 | 0.12 | 0.01 | 0.12 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HZ | 8 | 0.12 | 0.01 | 0.12 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HE1 | 8 | 0.12 | 0.01 | 0.12 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 8 | 0.12 | 0.01 | 0.12 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 8 | 0.11 | 0.01 | 0.11 |
| (2,339) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 7 | 0.67 | 0.18 | 0.61 |
| (2,339) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 7 | 0.67 | 0.18 | 0.61 |
| (2,339) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 7 | 0.67 | 0.18 | 0.61 |
| (4,338) | 1:111:A:LYS:HD3 | 1:104:A:LYS:HA | 7 | 0.54 | 0.11 | 0.51 |
| (2,3964) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H6N | 7 | 0.51 | 0.19 | 0.48 |
| (2,3415) | 1:122:A:VAL:HG21 | 1:122:A:VAL:H | 7 | 0.5 | 0.06 | 0.48 |
| (2,3415) | 1:122:A:VAL:HG22 | 1:122:A:VAL:H | 7 | 0.5 | 0.06 | 0.48 |
| (2,3415) | 1:122:A:VAL:HG23 | 1:122:A:VAL:H | 7 | 0.5 | 0.06 | 0.48 |
| (4,300) | 1:97:A:LEU:HD23 | 1:156:A:PHE:HB3 | 7 | 0.46 | 0.24 | 0.43 |
| (4,300) | 1:97:A:LEU:HD21 | 1:175:A:PHE:HB3 | 7 | 0.46 | 0.24 | 0.43 |
| (4,300) | 1:97:A:LEU:HD23 | 1:175:A:PHE:HB3 | 7 | 0.46 | 0.24 | 0.43 |
| (2,1276) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HE1 | 7 | 0.43 | 0.16 | 0.53 |
| (2,3459) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 7 | 0.41 | 0.17 | 0.37 |
| (2,3459) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 7 | 0.41 | 0.17 | 0.37 |
| (2,2308) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 7 | 0.33 | 0.18 | 0.27 |
| (2,2308) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 7 | 0.33 | 0.18 | 0.27 |
| (2,2308) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 7 | 0.33 | 0.18 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1288) | 1:167:A:LEU:HD22 | 1:167:A:LEU:HA | 7 | 0.3 | 0.09 | 0.25 |
| (2,1288) | 1:167:A:LEU:HD23 | 1:167:A:LEU:HA | 7 | 0.3 | 0.09 | 0.25 |
| (2,1459) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 7 | 0.3 | 0.1 | 0.29 |
| (2,1459) | 1:108:A:LEU:HD12 | 2:201:A:NAD:H2A | 7 | 0.3 | 0.1 | 0.29 |
| (2,1459) | 1:108:A:LEU:HD13 | 2:201:A:NAD:H2A | 7 | 0.3 | 0.1 | 0.29 |
| (2,3182) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 7 | 0.29 | 0.14 | 0.26 |
| (2,708) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 7 | 0.26 | 0.07 | 0.26 |
| (4,319) | 1:26:A:LEU:HD23 | 1:14:A:VAL:HA | 7 | 0.24 | 0.08 | 0.24 |
| (4,319) | 1:26:A:LEU:HD21 | 1:14:A:VAL:HA | 7 | 0.24 | 0.08 | 0.24 |
| (4,319) | 1:26:A:LEU:HD22 | 1:14:A:VAL:HA | 7 | 0.24 | 0.08 | 0.24 |
| (2,1563) | 1:48:A:ILE:HG23 | 1:53:A:LEU:HB2 | 7 | 0.23 | 0.07 | 0.23 |
| (2,1563) | 1:48:A:ILE:HG22 | 1:53:A:LEU:HB2 | 7 | 0.23 | 0.07 | 0.23 |
| (2,3829) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 7 | 0.22 | 0.06 | 0.21 |
| (2,1131) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 7 | 0.22 | 0.02 | 0.22 |
| (2,726) | 1:20:A:ALA:HB2 | 1:23:A:GLY:H | 7 | 0.2 | 0.03 | 0.19 |
| (2,550) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 7 | 0.2 | 0.05 | 0.21 |
| (2,550) | 1:105:A:ASN:H | 1:102:A:ALA:HB3 | 7 | 0.2 | 0.05 | 0.21 |
| (2,1172) | 1:144:A:LEU:HD11 | 1:106:A:PHE:HE1 | 7 | 0.19 | 0.04 | 0.2 |
| (1,92) | 1:133:A:LYS:N | 1:129:A:THR:O | 7 | 0.18 | 0.04 | 0.19 |
| (1,4) | 1:8:A:SER:N | 1:4:A:MET:O | 7 | 0.16 | 0.03 | 0.16 |
| (2,1973) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 7 | 0.14 | 0.01 | 0.15 |
| (2,431) | 1:73:A:LYS:H | 1:34:A:VAL:HG21 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1860) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 7 | 0.13 | 0.02 | 0.11 |
| (2,3180) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 7 | 0.11 | 0.01 | 0.11 |
| (2,1361) | 1:177:A:LYS:HE2 | 1:147:A:ASP:H | 6 | 1.5 | 0.46 | 1.52 |
| (2,1554) | 1:38:A:LEU:HD21 | 1:50:A:MET:HG2 | 6 | 0.75 | 0.17 | 0.78 |
| (2,3657) | 1:63:A:LYS:HG2 | 1:62:A:LYS:HA | 6 | 0.69 | 0.06 | 0.7 |
| (2,3657) | 1:63:A:LYS:HG3 | 1:62:A:LYS:HA | 6 | 0.69 | 0.06 | 0.7 |
| (2,1690) | 1:63:A:LYS:HG2 | 1:62:A:LYS:HA | 6 | 0.62 | 0.06 | 0.63 |
| (2,1690) | 1:63:A:LYS:HG3 | 1:62:A:LYS:HA | 6 | 0.62 | 0.06 | 0.63 |
| (2,3508) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 6 | 0.52 | 0.28 | 0.41 |
| (2,1831) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 6 | 0.52 | 0.15 | 0.59 |
| (2,1211) | 1:177:A:LYS:HD2 | 1:177:A:LYS:HA | 6 | 0.32 | 0.11 | 0.36 |
| (1,112) | 1:159:A:TYR:N | 1:167:A:LEU:O | 6 | 0.22 | 0.0 | 0.22 |
| (1,77) | 1:112:A:ASP:H | 1:108:A:LEU:O | 6 | 0.19 | 0.03 | 0.2 |
| (1,111) | 1:159:A:TYR:H | 1:167:A:LEU:O | 6 | 0.18 | 0.01 | 0.18 |
| (1,118) | 1:168:A:ILE:N | 1:122:A:VAL:O | 6 | 0.18 | 0.05 | 0.18 |
| (2,3345) | 1:41:A:MET:HE1 | 1:10:A:PHE:HE1 | 6 | 0.18 | 0.04 | 0.18 |
| (2,3345) | 1:41:A:MET:HE2 | 1:10:A:PHE:HE1 | 6 | 0.18 | 0.04 | 0.18 |
| (2,2657) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 6 | 0.16 | 0.04 | 0.16 |
| (2,3509) | 1:13:A:LEU:HD23 | 1:17:A:HIS:HB2 | 6 | 0.16 | 0.03 | 0.16 |
| (2,3509) | 1:13:A:LEU:HD21 | 1:17:A:HIS:HB2 | 6 | 0.16 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3509) | 1:13:A:LEU:HD22 | 1:17:A:HIS:HB2 | 6 | 0.16 | 0.03 | 0.16 |
| (1,24) | 1:37:A:LEU:N | 1:33:A:PRO:O | 6 | 0.15 | 0.03 | 0.15 |
| (2,268) | 1:14:A:VAL:HG21 | 1:21:A:LEU:H | 6 | 0.14 | 0.03 | 0.14 |
| (2,268) | 1:14:A:VAL:HG22 | 1:21:A:LEU:H | 6 | 0.14 | 0.03 | 0.14 |
| (2,268) | 1:14:A:VAL:HG23 | 1:21:A:LEU:H | 6 | 0.14 | 0.03 | 0.14 |
| (2,1432) | 1:38:A:LEU:HD12 | 1:39:A:ALA:H | 6 | 0.13 | 0.03 | 0.12 |
| (2,1432) | 1:38:A:LEU:HD13 | 1:39:A:ALA:H | 6 | 0.13 | 0.03 | 0.12 |
| (2,1432) | 1:38:A:LEU:HD11 | 1:39:A:ALA:H | 6 | 0.13 | 0.03 | 0.12 |
| (2,2651) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE22 | 6 | 0.13 | 0.0 | 0.13 |
| (2,1110) | 1:76:A:ALA:H | 1:75:A:ARG:H | 6 | 0.13 | 0.03 | 0.12 |
| (2,3468) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HA | 6 | 0.12 | 0.01 | 0.12 |
| (2,3468) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HA | 6 | 0.12 | 0.01 | 0.12 |
| (2,62) | 1:178:A:VAL:H | 1:177:A:LYS:H | 6 | 0.11 | 0.01 | 0.11 |
| (2,2010) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 6 | 0.11 | 0.01 | 0.11 |
| (2,3173) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 6 | 0.1 | 0.0 | 0.11 |
| (2,1840) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG22 | 5 | 0.6 | 0.06 | 0.62 |
| (2,1840) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG21 | 5 | 0.6 | 0.06 | 0.62 |
| (2,1840) | 1:128:A:ILE:HG23 | 1:129:A:THR:HG21 | 5 | 0.6 | 0.06 | 0.62 |
| (4,409) | 1:4:A:MET:HE1 | 1:59:A:THR:HG23 | 5 | 0.47 | 0.21 | 0.52 |
| (4,409) | 1:4:A:MET:HE3 | 1:59:A:THR:HG23 | 5 | 0.47 | 0.21 | 0.52 |
| (4,299) | 1:168:A:ILE:HD12 | 1:152:A:ALA:HA | 5 | 0.37 | 0.16 | 0.36 |
| (4,299) | 1:168:A:ILE:HD12 | 1:96:A:VAL:HA | 5 | 0.37 | 0.16 | 0.36 |
| (4,299) | 1:168:A:ILE:HD11 | 1:96:A:VAL:HA | 5 | 0.37 | 0.16 | 0.36 |
| (2,19) | 1:13:A:LEU:HA | 1:17:A:HIS:HD2 | 5 | 0.36 | 0.12 | 0.43 |
| (2,3791) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 5 | 0.35 | 0.09 | 0.38 |
| (2,1555) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 5 | 0.35 | 0.12 | 0.36 |
| (2,1555) | 1:84:A:VAL:HG21 | 1:85:A:ASP:HB2 | 5 | 0.35 | 0.12 | 0.36 |
| (2,3804) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG22 | 5 | 0.28 | 0.06 | 0.3 |
| (2,3804) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG21 | 5 | 0.28 | 0.06 | 0.3 |
| (2,3804) | 1:128:A:ILE:HG23 | 1:129:A:THR:HG21 | 5 | 0.28 | 0.06 | 0.3 |
| (2,120) | 1:177:A:LYS:HB3 | 1:178:A:VAL:H | 5 | 0.26 | 0.02 | 0.25 |
| (2,3789) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HB3 | 5 | 0.24 | 0.08 | 0.23 |
| (2,3785) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 5 | 0.22 | 0.09 | 0.2 |
| (2,3785) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 5 | 0.22 | 0.09 | 0.2 |
| (2,1420) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HE1 | 5 | 0.22 | 0.05 | 0.21 |
| (2,1420) | 1:22:A:ILE:HG21 | 1:10:A:PHE:HE1 | 5 | 0.22 | 0.05 | 0.21 |
| (4,443) | 1:48:A:ILE:HD12 | 1:38:A:LEU:HB2 | 5 | 0.22 | 0.06 | 0.21 |
| (4,443) | 1:48:A:ILE:HD13 | 1:38:A:LEU:HB2 | 5 | 0.22 | 0.06 | 0.21 |
| (2,1218) | 1:177:A:LYS:HG2 | 1:177:A:LYS:HA | 5 | 0.2 | 0.03 | 0.19 |
| (2,3940) | 1:134:A:VAL:HG11 | 2:201:A:NAD:H2N | 5 | 0.17 | 0.03 | 0.17 |
| (1,88) | 1:131:A:ALA:N | 1:127:A:ASP:O | 5 | 0.16 | 0.04 | 0.13 |
| (4,8) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HD1 | 5 | 0.15 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,2175) | 1:57:A:VAL:HG21 | 1:66:A:ALA:H | 5 | 0.15 | 0.04 | 0.13 |
| (2,2175) | 1:57:A:VAL:HG22 | 1:66:A:ALA:H | 5 | 0.15 | 0.04 | 0.13 |
| (1,89) | 1:132:A:ARG:H | 1:128:A:ILE:O | 5 | 0.14 | 0.02 | 0.13 |
| (1,119) | 1:171:A:VAL:H | 1:114:A:ILE:O | 5 | 0.13 | 0.03 | 0.12 |
| (1,55) | 1:74:A:ILE:H | 1:32:A:ALA:O | 5 | 0.13 | 0.01 | 0.12 |
| (2,2192) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 5 | 0.13 | 0.02 | 0.12 |
| (2,3478) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 5 | 0.12 | 0.01 | 0.12 |
| (2,3478) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 5 | 0.12 | 0.01 | 0.12 |
| (2,3825) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB2 | 5 | 0.12 | 0.02 | 0.12 |
| (2,3825) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB2 | 5 | 0.12 | 0.02 | 0.12 |
| (4,65) | 1:7:A:VAL:H | 1:7:A:VAL:HB | 5 | 0.12 | 0.01 | 0.12 |
| (4,65) | 1:6:A:LYS:HB3 | 1:7:A:VAL:H | 5 | 0.12 | 0.01 | 0.12 |
| (2,2520) | 1:8:A:SER:H | 1:6:A:LYS:HA | 5 | 0.12 | 0.02 | 0.1 |
| (2,2887) | 1:176:A:ILE:H | 1:146:A:VAL:HG11 | 5 | 0.12 | 0.01 | 0.11 |
| (1,39) | 1:54:A:LYS:H | 1:50:A:MET:O | 5 | 0.11 | 0.01 | 0.12 |
| (2,3775) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 5 | 0.11 | 0.0 | 0.11 |
| (2,42) | 1:148:A:ALA:H | 1:148:A:ALA:HB1 | 5 | 0.11 | 0.0 | 0.11 |
| (2,950) | 1:76:A:ALA:H | 1:76:A:ALA:HA | 5 | 0.11 | 0.0 | 0.11 |
| (2,2980) | 1:40:A:LYS:H | 1:39:A:ALA:H | 5 | 0.11 | 0.0 | 0.11 |
| (2,1217) | 1:177:A:LYS:HE2 | 1:177:A:LYS:HB2 | 4 | 1.18 | 0.31 | 1.09 |
| (4,313) | 1:143:A:VAL:HG12 | 1:145:A:SER:HA | 4 | 0.97 | 0.11 | 0.98 |
| (4,313) | 1:96:A:VAL:HG13 | 1:145:A:SER:HA | 4 | 0.97 | 0.11 | 0.98 |
| (2,1794) | 1:117:A:MET:HE1 | 1:117:A:MET:HB2 | 4 | 0.55 | 0.19 | 0.55 |
| (2,1794) | 1:117:A:MET:HE3 | 1:117:A:MET:HB2 | 4 | 0.55 | 0.19 | 0.55 |
| (2,3500) | 1:144:A:LEU:HD22 | 1:145:A:SER:HB2 | 4 | 0.52 | 0.4 | 0.47 |
| (2,3500) | 1:144:A:LEU:HD21 | 1:145:A:SER:HB2 | 4 | 0.52 | 0.4 | 0.47 |
| (2,3500) | 1:144:A:LEU:HD23 | 1:145:A:SER:HB2 | 4 | 0.52 | 0.4 | 0.47 |
| (2,948) | 1:76:A:ALA:HB1 | 1:78:A:GLN:HE22 | 4 | 0.48 | 0.21 | 0.57 |
| (2,948) | 1:76:A:ALA:HB3 | 1:78:A:GLN:HE22 | 4 | 0.48 | 0.21 | 0.57 |
| (2,3722) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 4 | 0.48 | 0.22 | 0.6 |
| (2,3177) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 4 | 0.47 | 0.06 | 0.44 |
| (2,305) | 1:42:A:LYS:HA | 1:46:A:HIS:H | 4 | 0.46 | 0.21 | 0.57 |
| (2,3761) | 1:117:A:MET:HE1 | 1:117:A:MET:HB2 | 4 | 0.44 | 0.19 | 0.44 |
| (2,3761) | 1:117:A:MET:HE3 | 1:117:A:MET:HB2 | 4 | 0.44 | 0.19 | 0.44 |
| (2,29) | 1:88:A:TYR:HD1 | 1:159:A:TYR:HD1 | 4 | 0.43 | 0.04 | 0.42 |
| (4,227) | 1:8:A:SER:HB3 | 1:65:A:PHE:HE1 | 4 | 0.41 | 0.24 | 0.41 |
| (4,227) | 1:8:A:SER:HB3 | 1:55:A:HIS:HD2 | 4 | 0.41 | 0.24 | 0.41 |
| (2,342) | 1:41:A:MET:H | 1:41:A:MET:HG2 | 4 | 0.41 | 0.25 | 0.42 |
| (2,1511) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 4 | 0.4 | 0.28 | 0.38 |
| (2,3481) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 4 | 0.4 | 0.28 | 0.37 |
| (4,70) | 1:130:A:THR:H | 2:201:A:NAD:H4D | 4 | 0.36 | 0.2 | 0.34 |
| (2,1588) | 1:152:A:ALA:HB2 | 1:149:A:LYS:HA | 4 | 0.29 | 0.15 | 0.3 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,2738) | 1:30:A:GLY:H | 1:26:A:LEU:HD23 | 4 | 0.28 | 0.11 | 0.3 |
| (2,2738) | 1:30:A:GLY:H | 1:26:A:LEU:HD21 | 4 | 0.28 | 0.11 | 0.3 |
| (2,2738) | 1:30:A:GLY:H | 1:26:A:LEU:HD22 | 4 | 0.28 | 0.11 | 0.3 |
| (2,2748) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 4 | 0.27 | 0.13 | 0.28 |
| (2,3355) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 4 | 0.27 | 0.13 | 0.23 |
| (2,3430) | 1:128:A:ILE:HD11 | 1:127:A:ASP:H | 4 | 0.26 | 0.1 | 0.2 |
| (2,3430) | 1:128:A:ILE:HD12 | 1:127:A:ASP:H | 4 | 0.26 | 0.1 | 0.2 |
| (2,3430) | 1:128:A:ILE:HD13 | 1:127:A:ASP:H | 4 | 0.26 | 0.1 | 0.2 |
| (2,985) | 1:46:A:HIS:H | 1:45:A:GLY:H | 4 | 0.24 | 0.01 | 0.24 |
| (2,3531) | 1:151:A:MET:HE1 | 1:175:A:PHE:HB3 | 4 | 0.23 | 0.05 | 0.21 |
| (2,3531) | 1:151:A:MET:HE2 | 1:175:A:PHE:HB3 | 4 | 0.23 | 0.05 | 0.21 |
| (2,1075) | 1:56:A:ILE:H | 1:58:A:GLU:H | 4 | 0.22 | 0.06 | 0.21 |
| (2,1889) | 1:4:A:MET:HE1 | 1:4:A:MET:HA | 4 | 0.2 | 0.03 | 0.18 |
| (2,718) | 1:91:A:GLN:HE21 | 1:89:A:GLU:HB2 | 4 | 0.19 | 0.01 | 0.19 |
| (2,2417) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 4 | 0.19 | 0.03 | 0.18 |
| (2,1590) | 1:32:A:ALA:HB2 | 1:33:A:PRO:HD3 | 4 | 0.17 | 0.07 | 0.14 |
| (2,224) | 1:81:A:SER:HA | 1:82:A:VAL:H | 4 | 0.16 | 0.04 | 0.16 |
| (2,2189) | 1:81:A:SER:HA | 1:82:A:VAL:H | 4 | 0.15 | 0.04 | 0.15 |
| (2,3920) | 1:115:A:LYS:H | 2:201:A:NAD:H8A | 4 | 0.14 | 0.03 | 0.14 |
| (2,453) | 1:34:A:VAL:HB | 1:35:A:LYS:H | 4 | 0.13 | 0.02 | 0.14 |
| (2,2649) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 4 | 0.12 | 0.01 | 0.12 |
| (2,3102) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 4 | 0.12 | 0.01 | 0.12 |
| (1,97) | 1:136:A:MET:H | 1:132:A:ARG:O | 4 | 0.12 | 0.01 | 0.12 |
| (2,3036) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 4 | 0.12 | 0.01 | 0.12 |
| (2,3924) | 1:109:A:ILE:HD11 | 2:201:A:NAD:H2A | 4 | 0.12 | 0.01 | 0.12 |
| (2,1964) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HD1 | 4 | 0.11 | 0.01 | 0.11 |
| (2,3712) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 4 | 0.11 | 0.0 | 0.11 |
| (2,3712) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 4 | 0.11 | 0.0 | 0.11 |
| (2,3184) | 1:92:A:VAL:HG21 | 1:92:A:VAL:H | 4 | 0.1 | 0.0 | 0.1 |
| (2,3197) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 4 | 0.1 | 0.0 | 0.1 |
| (2,1984) | 1:106:A:PHE:HD1 | 1:106:A:PHE:HE1 | 4 | 0.1 | 0.0 | 0.1 |
| (2,1236) | 1:151:A:MET:HE2 | 1:156:A:PHE:HZ | 3 | 1.02 | 0.23 | 0.93 |
| (2,1236) | 1:151:A:MET:HE3 | 1:156:A:PHE:HZ | 3 | 1.02 | 0.23 | 0.93 |
| (2,1236) | 1:151:A:MET:HE1 | 1:156:A:PHE:HZ | 3 | 1.02 | 0.23 | 0.93 |
| (2,32) | 1:88:A:TYR:HE1 | 1:159:A:TYR:HD1 | 3 | 0.9 | 0.74 | 0.46 |
| (4,160) | 1:22:A:ILE:HD12 | 1:22:A:ILE:H | 3 | 0.75 | 0.02 | 0.75 |
| (4,160) | 1:22:A:ILE:HD11 | 1:22:A:ILE:H | 3 | 0.75 | 0.02 | 0.75 |
| (4,160) | 1:22:A:ILE:HD13 | 1:22:A:ILE:H | 3 | 0.75 | 0.02 | 0.75 |
| (4,301) | 1:97:A:LEU:HD23 | 1:156:A:PHE:HB2 | 3 | 0.65 | 0.22 | 0.52 |
| (4,301) | 1:97:A:LEU:HD22 | 1:156:A:PHE:HB2 | 3 | 0.65 | 0.22 | 0.52 |
| (4,301) | 1:97:A:LEU:HD23 | 1:175:A:PHE:HB2 | 3 | 0.65 | 0.22 | 0.52 |
| (2,1535) | 1:22:A:ILE:HG21 | 1:44:A:LYS:HE3 | 3 | 0.61 | 0.26 | 0.67 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,1535) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HE3 | 3 | 0.61 | 0.26 | 0.67 |
| (2,2266) | 1:153:A:ASP:H | 1:95:A:ALA:HB1 | 3 | 0.57 | 0.27 | 0.56 |
| (2,3839) | 1:129:A:THR:HG22 | 1:129:A:THR:HA | 3 | 0.56 | 0.03 | 0.55 |
| (2,3839) | 1:129:A:THR:HG21 | 1:129:A:THR:HA | 3 | 0.56 | 0.03 | 0.55 |
| (2,1426) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HD1 | 3 | 0.48 | 0.19 | 0.44 |
| (2,1426) | 1:86:A:LEU:HD12 | 1:88:A:TYR:HD1 | 3 | 0.48 | 0.19 | 0.44 |
| (2,1877) | 1:129:A:THR:HG22 | 1:129:A:THR:HA | 3 | 0.47 | 0.03 | 0.46 |
| (2,1877) | 1:129:A:THR:HG21 | 1:129:A:THR:HA | 3 | 0.47 | 0.03 | 0.46 |
| (2,300) | 1:153:A:ASP:H | 1:95:A:ALA:HB1 | 3 | 0.45 | 0.27 | 0.44 |
| (2,1412) | 1:66:A:ALA:HB2 | 1:31:A:TRP:HZ3 | 3 | 0.41 | 0.19 | 0.35 |
| (2,3211) | 1:151:A:MET:HE2 | 1:156:A:PHE:HZ | 3 | 0.37 | 0.24 | 0.28 |
| (2,3211) | 1:151:A:MET:HE3 | 1:156:A:PHE:HZ | 3 | 0.37 | 0.24 | 0.28 |
| (2,3211) | 1:151:A:MET:HE1 | 1:156:A:PHE:HZ | 3 | 0.37 | 0.24 | 0.28 |
| (2,3378) | 1:66:A:ALA:HB2 | 1:31:A:TRP:HZ3 | 3 | 0.36 | 0.19 | 0.31 |
| (2,629) | 1:44:A:LYS:H | 1:42:A:LYS:HG3 | 3 | 0.31 | 0.01 | 0.31 |
| (4,364) | 1:4:A:MET:HE2 | 1:58:A:GLU:HG3 | 3 | 0.29 | 0.07 | 0.25 |
| (4,364) | 1:4:A:MET:HE3 | 1:58:A:GLU:HG3 | 3 | 0.29 | 0.07 | 0.25 |
| (4,364) | 1:4:A:MET:HE2 | 1:53:A:LEU:HB2 | 3 | 0.29 | 0.07 | 0.25 |
| (4,195) | 1:114:A:ILE:HD11 | 1:117:A:MET:HE1 | 3 | 0.29 | 0.11 | 0.3 |
| (2,2625) | 1:29:A:ASN:H | 1:29:A:ASN:HB3 | 3 | 0.25 | 0.0 | 0.25 |
| (2,653) | 1:29:A:ASN:H | 1:29:A:ASN:HB3 | 3 | 0.24 | 0.0 | 0.24 |
| (2,1754) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 3 | 0.23 | 0.0 | 0.23 |
| (2,2918) | 1:76:A:ALA:HB1 | 1:78:A:GLN:HE22 | 3 | 0.23 | 0.04 | 0.22 |
| (2,2918) | 1:76:A:ALA:HB3 | 1:78:A:GLN:HE22 | 3 | 0.23 | 0.04 | 0.22 |
| (2,1014) | 1:160:A:LEU:H | 1:89:A:GLU:H | 3 | 0.22 | 0.07 | 0.19 |
| (2,1155) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 3 | 0.21 | 0.03 | 0.22 |
| (4,453) | 1:48:A:ILE:HG13 | 1:38:A:LEU:HA | 3 | 0.21 | 0.03 | 0.22 |
| (2,3559) | 1:102:A:ALA:HB1 | 2:201:A:NAD:H4B | 3 | 0.19 | 0.07 | 0.17 |
| (2,3679) | 1:97:A:LEU:HD21 | 1:97:A:LEU:HA | 3 | 0.19 | 0.09 | 0.15 |
| (2,3679) | 1:97:A:LEU:HD23 | 1:97:A:LEU:HA | 3 | 0.19 | 0.09 | 0.15 |
| (1,117) | 1:168:A:ILE:H | 1:122:A:VAL:O | 3 | 0.18 | 0.02 | 0.19 |
| (2,2949) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 3 | 0.18 | 0.09 | 0.14 |
| (2,3959) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H5N | 3 | 0.18 | 0.06 | 0.16 |
| (1,2) | 1:7:A:VAL:N | 1:3:A:HIS:O | 3 | 0.16 | 0.02 | 0.16 |
| (2,2232) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 3 | 0.16 | 0.02 | 0.17 |
| (2,2232) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 3 | 0.16 | 0.02 | 0.17 |
| (4,213) | 1:165:A:VAL:HB | 1:123:A:HIS:HA | 3 | 0.15 | 0.04 | 0.13 |
| (4,213) | 1:143:A:VAL:HB | 1:144:A:LEU:HA | 3 | 0.15 | 0.04 | 0.13 |
| (2,2234) | 1:14:A:VAL:HG23 | 1:21:A:LEU:H | 3 | 0.14 | 0.02 | 0.14 |
| (2,2234) | 1:14:A:VAL:HG22 | 1:21:A:LEU:H | 3 | 0.14 | 0.02 | 0.14 |
| (2,2680) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 3 | 0.14 | 0.05 | 0.11 |
| (2,1158) | 1:165:A:VAL:HG21 | 1:165:A:VAL:H | 3 | 0.14 | 0.0 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,9) | 1:11:A:LEU:H | 1:7:A:VAL:O | 3 | 0.13 | 0.0 | 0.13 |
| (1,110) | 1:153:A:ASP:N | 1:149:A:LYS:O | 3 | 0.13 | 0.01 | 0.12 |
| (2,1399) | 1:86:A:LEU:HG | 1:86:A:LEU:H | 3 | 0.13 | 0.02 | 0.14 |
| (2,96) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 3 | 0.13 | 0.02 | 0.12 |
| (2,673) | 1:70:A:ASN:HD22 | 1:50:A:MET:HG3 | 3 | 0.13 | 0.04 | 0.1 |
| (2,1745) | 1:34:A:VAL:HA | 1:37:A:LEU:HD21 | 3 | 0.13 | 0.02 | 0.13 |
| (2,3884) | 2:201:A:NAD:H1B | 1:109:A:ILE:HD12 | 3 | 0.13 | 0.02 | 0.12 |
| (1,59) | 1:77:A:ASN:H | 1:64:A:ARG:O | 3 | 0.12 | 0.03 | 0.11 |
| (1,91) | 1:133:A:LYS:H | 1:129:A:THR:O | 3 | 0.12 | 0.0 | 0.12 |
| (2,54) | 1:34:A:VAL:H | 1:74:A:ILE:HG21 | 3 | 0.12 | 0.01 | 0.13 |
| (2,54) | 1:34:A:VAL:H | 1:74:A:ILE:HG22 | 3 | 0.12 | 0.01 | 0.13 |
| (2,904) | 1:92:A:VAL:H | 1:92:A:VAL:HA | 3 | 0.12 | 0.0 | 0.12 |
| (2,445) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 3 | 0.12 | 0.02 | 0.11 |
| (2,1842) | 1:11:A:LEU:HD21 | 1:11:A:LEU:HB2 | 3 | 0.12 | 0.01 | 0.13 |
| (2,1842) | 1:11:A:LEU:HD22 | 1:11:A:LEU:HB2 | 3 | 0.12 | 0.01 | 0.13 |
| (2,2722) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 3 | 0.12 | 0.01 | 0.12 |
| (2,3295) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 3 | 0.12 | 0.0 | 0.12 |
| (4,425) | 1:34:A:VAL:HG21 | 1:35:A:LYS:HB2 | 3 | 0.12 | 0.02 | 0.11 |
| (2,1308) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HA | 3 | 0.11 | 0.0 | 0.11 |
| (2,2492) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 3 | 0.11 | 0.01 | 0.11 |
| (2,2492) | 1:129:A:THR:HG22 | 1:129:A:THR:H | 3 | 0.11 | 0.01 | 0.11 |
| (2,1207) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 3 | 0.11 | 0.01 | 0.1 |
| (2,3764) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 3 | 0.11 | 0.0 | 0.11 |
| (2,1733) | 1:7:A:VAL:HA | 1:7:A:VAL:HB | 3 | 0.1 | 0.0 | 0.1 |
| (2,1610) | 1:13:A:LEU:HG | 1:17:A:HIS:HB2 | 2 | 0.78 | 0.04 | 0.78 |
| (2,1529) | 1:144:A:LEU:HD22 | 1:145:A:SER:HB2 | 2 | 0.75 | 0.12 | 0.75 |
| (2,1529) | 1:144:A:LEU:HD23 | 1:145:A:SER:HB2 | 2 | 0.75 | 0.12 | 0.75 |
| (4,402) | 1:6:A:LYS:HE2 | 1:6:A:LYS:HG3 | 2 | 0.73 | 0.01 | 0.73 |
| (4,402) | 1:42:A:LYS:HG3 | 1:42:A:LYS:HE3 | 2 | 0.73 | 0.01 | 0.73 |
| (4,9) | 1:22:A:ILE:HD13 | 1:10:A:PHE:HD1 | 2 | 0.58 | 0.35 | 0.58 |
| (4,9) | 1:10:A:PHE:HD1 | 1:7:A:VAL:HG11 | 2 | 0.58 | 0.35 | 0.58 |
| (2,1846) | 1:160:A:LEU:HD13 | 1:91:A:GLN:HB2 | 2 | 0.56 | 0.06 | 0.56 |
| (2,1846) | 1:160:A:LEU:HD11 | 1:91:A:GLN:HB2 | 2 | 0.56 | 0.06 | 0.56 |
| (2,3788) | 1:151:A:MET:HE1 | 1:151:A:MET:HG3 | 2 | 0.52 | 0.02 | 0.52 |
| (2,3788) | 1:151:A:MET:HE2 | 1:151:A:MET:HG3 | 2 | 0.52 | 0.02 | 0.52 |
| (2,2348) | 1:156:A:PHE:H | 1:168:A:ILE:HD12 | 2 | 0.52 | 0.29 | 0.52 |
| (2,2348) | 1:156:A:PHE:H | 1:168:A:ILE:HD11 | 2 | 0.52 | 0.29 | 0.52 |
| (2,3843) | 1:76:A:ALA:HB1 | 1:16:A:ARG:HA | 2 | 0.51 | 0.05 | 0.51 |
| (2,3843) | 1:76:A:ALA:HB3 | 1:16:A:ARG:HA | 2 | 0.51 | 0.05 | 0.51 |
| (4,129) | 1:13:A:LEU:HD23 | 1:18:A:ASN:H | 2 | 0.48 | 0.04 | 0.48 |
| (4,129) | 1:13:A:LEU:HD21 | 1:18:A:ASN:H | 2 | 0.48 | 0.04 | 0.48 |
| (2,2221) | 1:168:A:ILE:HD12 | 1:157:A:ASP:H | 2 | 0.45 | 0.35 | 0.45 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,3461) | 1:168:A:ILE:HD12 | 1:156:A:PHE:HB2 | 2 | 0.41 | 0.12 | 0.41 |
| (2,3461) | 1:168:A:ILE:HD11 | 1:156:A:PHE:HB2 | 2 | 0.41 | 0.12 | 0.41 |
| (4,410) | 1:50:A:MET:HE3 | 1:54:A:LYS:HD3 | 2 | 0.4 | 0.18 | 0.4 |
| (4,410) | 1:50:A:MET:HE3 | 1:54:A:LYS:HD2 | 2 | 0.4 | 0.18 | 0.4 |
| (4,223) | 1:13:A:LEU:HD12 | 1:10:A:PHE:HE1 | 2 | 0.36 | 0.21 | 0.36 |
| (2,3446) | 1:74:A:ILE:HD12 | 1:67:A:PHE:HE1 | 2 | 0.33 | 0.22 | 0.33 |
| (2,3384) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HD22 | 2 | 0.32 | 0.02 | 0.32 |
| (4,322) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 2 | 0.32 | 0.02 | 0.32 |
| (2,2123) | 1:86:A:LEU:H | 1:86:A:LEU:HB3 | 2 | 0.27 | 0.02 | 0.27 |
| (4,411) | 1:84:A:VAL:HB | 1:86:A:LEU:HB3 | 2 | 0.27 | 0.06 | 0.27 |
| (4,411) | 1:172:A:PRO:HB2 | 1:114:A:ILE:HG12 | 2 | 0.27 | 0.06 | 0.27 |
| (4,387) | 1:83:A:GLU:HA | 1:82:A:VAL:HG12 | 2 | 0.26 | 0.08 | 0.26 |
| (4,40) | 1:5:A:VAL:H | 1:5:A:VAL:HB | 2 | 0.26 | 0.0 | 0.26 |
| (2,164) | 1:86:A:LEU:H | 1:86:A:LEU:HB3 | 2 | 0.26 | 0.03 | 0.26 |
| (2,1274) | 1:160:A:LEU:HD22 | 1:91:A:GLN:HE22 | 2 | 0.25 | 0.1 | 0.25 |
| (2,1274) | 1:160:A:LEU:HD21 | 1:91:A:GLN:HE22 | 2 | 0.25 | 0.1 | 0.25 |
| (2,486) | 1:58:A:GLU:H | 1:58:A:GLU:HB3 | 2 | 0.24 | 0.01 | 0.24 |
| (2,3248) | 1:160:A:LEU:HD22 | 1:91:A:GLN:HE22 | 2 | 0.24 | 0.1 | 0.24 |
| (2,3248) | 1:160:A:LEU:HD21 | 1:91:A:GLN:HE22 | 2 | 0.24 | 0.1 | 0.24 |
| (2,768) | 1:30:A:GLY:H | 1:26:A:LEU:HD21 | 2 | 0.22 | 0.04 | 0.22 |
| (2,768) | 1:30:A:GLY:H | 1:26:A:LEU:HD22 | 2 | 0.22 | 0.04 | 0.22 |
| (2,1208) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 2 | 0.22 | 0.1 | 0.22 |
| (2,3558) | 1:152:A:ALA:HB2 | 1:149:A:LYS:HA | 2 | 0.21 | 0.01 | 0.21 |
| (2,1633) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 2 | 0.2 | 0.06 | 0.2 |
| (1,18) | 1:15:A:LEU:N | 1:11:A:LEU:O | 2 | 0.2 | 0.0 | 0.2 |
| (2,190) | 1:13:A:LEU:H | 1:13:A:LEU:HB3 | 2 | 0.19 | 0.01 | 0.19 |
| (2,1828) | 1:151:A:MET:HE1 | 1:151:A:MET:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (2,1828) | 1:151:A:MET:HE2 | 1:151:A:MET:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (2,2852) | 1:85:A:ASP:H | 1:86:A:LEU:H | 2 | 0.18 | 0.02 | 0.18 |
| (2,1880) | 1:76:A:ALA:HB1 | 1:16:A:ARG:HA | 2 | 0.18 | 0.04 | 0.18 |
| (2,1880) | 1:76:A:ALA:HB3 | 1:16:A:ARG:HA | 2 | 0.18 | 0.04 | 0.18 |
| (4,392) | 1:8:A:SER:HB2 | 1:7:A:VAL:HB | 2 | 0.17 | 0.03 | 0.17 |
| (2,811) | 1:14:A:VAL:HG23 | 1:22:A:ILE:H | 2 | 0.17 | 0.07 | 0.17 |
| (2,811) | 1:14:A:VAL:HG21 | 1:22:A:ILE:H | 2 | 0.17 | 0.07 | 0.17 |
| (1,17) | 1:15:A:LEU:H | 1:11:A:LEU:O | 2 | 0.16 | 0.02 | 0.16 |
| (2,2506) | 1:64:A:ARG:H | 1:76:A:ALA:HB1 | 2 | 0.16 | 0.03 | 0.16 |
| (2,2506) | 1:64:A:ARG:H | 1:76:A:ALA:HB3 | 2 | 0.16 | 0.03 | 0.16 |
| (4,448) | 1:110:A:LEU:HD21 | 1:144:A:LEU:HG | 2 | 0.16 | 0.01 | 0.16 |
| (4,448) | 1:110:A:LEU:HD22 | 1:144:A:LEU:HG | 2 | 0.16 | 0.01 | 0.16 |
| (2,3445) | 1:97:A:LEU:HD23 | 1:166:A:TRP:HE3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,3445) | 1:97:A:LEU:HD21 | 1:166:A:TRP:HE3 | 2 | 0.16 | 0.01 | 0.16 |
| (1,94) | 1:134:A:VAL:N | 1:130:A:THR:O | 2 | 0.15 | 0.03 | 0.15 |

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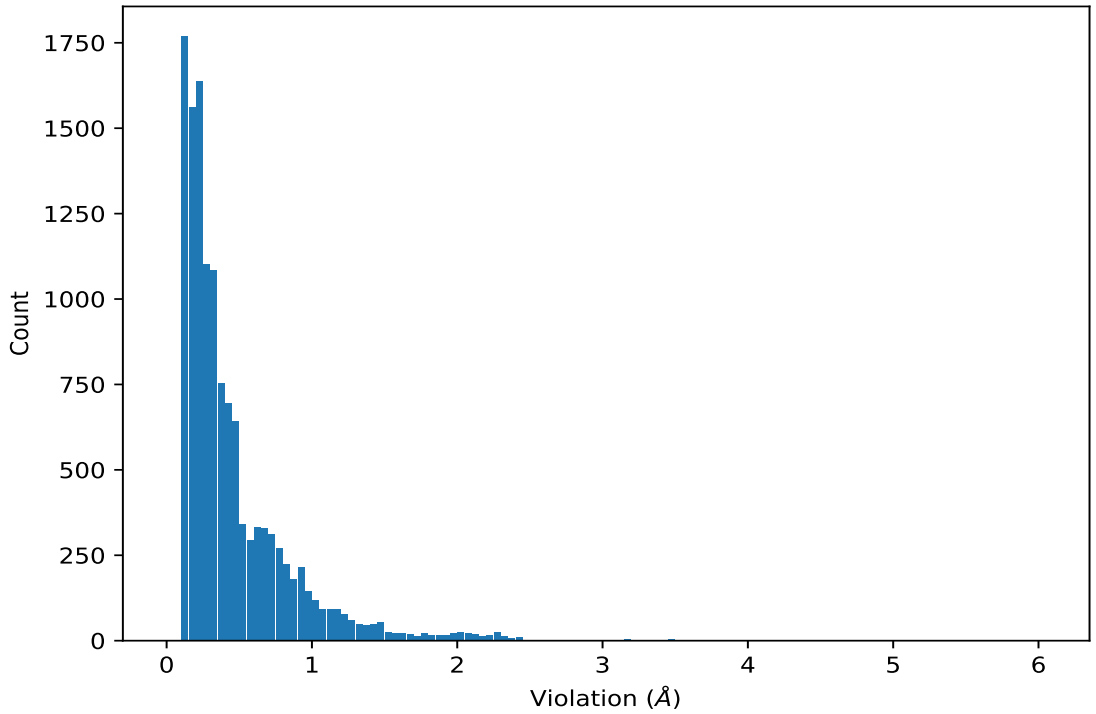
| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (2,61) | 1:166:A:TRP:HE1 | 1:126:A:GLN:HB2 | 2 | 0.15 | 0.04 | 0.15 |
| (2,184) | 1:26:A:LEU:H | 1:19:A:PRO:HA | 2 | 0.15 | 0.03 | 0.15 |
| (2,1932) | 2:201:A:NAD:H3D | 2:201:A:NAD:H2N | 2 | 0.15 | 0.02 | 0.15 |
| (2,3896) | 2:201:A:NAD:H3D | 2:201:A:NAD:H2N | 2 | 0.15 | 0.02 | 0.15 |
| (2,198) | 1:20:A:ALA:HA | 1:24:A:LEU:H | 2 | 0.14 | 0.01 | 0.14 |
| (4,209) | 1:76:A:ALA:HB3 | 1:16:A:ARG:H | 2 | 0.14 | 0.02 | 0.14 |
| (4,209) | 1:76:A:ALA:HB1 | 1:16:A:ARG:H | 2 | 0.14 | 0.02 | 0.14 |
| (2,723) | 1:20:A:ALA:HA | 1:23:A:GLY:H | 2 | 0.14 | 0.01 | 0.14 |
| (2,1591) | 1:95:A:ALA:HB1 | 1:149:A:LYS:HA | 2 | 0.14 | 0.02 | 0.14 |
| (2,3918) | 1:114:A:ILE:HD11 | 2:201:A:NAD:H8A | 2 | 0.14 | 0.01 | 0.14 |
| (2,43) | 1:96:A:VAL:HG21 | 1:148:A:ALA:H | 2 | 0.12 | 0.01 | 0.12 |
| (2,1099) | 1:100:A:GLY:H | 1:166:A:TRP:H | 2 | 0.12 | 0.01 | 0.12 |
| (2,2151) | 1:13:A:LEU:H | 1:13:A:LEU:HB3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,2216) | 1:26:A:LEU:HD11 | 1:27:A:ASP:H | 2 | 0.12 | 0.02 | 0.12 |
| (2,2216) | 1:26:A:LEU:HD13 | 1:27:A:ASP:H | 2 | 0.12 | 0.02 | 0.12 |
| (2,3947) | 1:165:A:VAL:HG21 | 2:201:A:NAD:H4N | 2 | 0.12 | 0.01 | 0.12 |
| (1,121) | 1:175:A:PHE:H | 1:172:A:PRO:O | 2 | 0.12 | 0.0 | 0.12 |
| (2,2550) | 1:86:A:LEU:H | 1:88:A:TYR:H | 2 | 0.12 | 0.01 | 0.12 |
| (2,3335) | 1:16:A:ARG:HD2 | 1:12:A:SER:H | 2 | 0.12 | 0.01 | 0.12 |
| (3,20) | 1:163:A:ASN:OD1 | 2:201:A:NAD:H71N | 2 | 0.12 | 0.02 | 0.12 |
| (2,99) | 1:140:A:LYS:H | 1:103:A:GLU:HA | 2 | 0.12 | 0.0 | 0.12 |
| (2,1687) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 2 | 0.11 | 0.01 | 0.11 |
| (2,1989) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 2 | 0.11 | 0.0 | 0.11 |
| (2,2132) | 1:56:A:ILE:HD11 | 1:56:A:ILE:H | 2 | 0.11 | 0.01 | 0.11 |
| (2,2212) | 1:53:A:LEU:H | 1:48:A:ILE:HG12 | 2 | 0.11 | 0.01 | 0.11 |
| (2,2269) | 1:84:A:VAL:HA | 1:84:A:VAL:H | 2 | 0.11 | 0.0 | 0.11 |
| (2,2305) | 1:173:A:ALA:HB1 | 1:176:A:ILE:H | 2 | 0.11 | 0.0 | 0.11 |
| (2,2597) | 1:44:A:LYS:H | 1:21:A:LEU:HA | 2 | 0.11 | 0.0 | 0.11 |
| (2,439) | 1:55:A:HIS:H | 1:54:A:LYS:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (2,3302) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 2 | 0.11 | 0.0 | 0.11 |
| (2,2822) | 1:74:A:ILE:H | 1:73:A:LYS:HB2 | 2 | 0.1 | 0.0 | 0.1 |

[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) |
|---|---|---|---|---|
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 2 | 6.05 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 14 | 5.97 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 9 | 5.03 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 16 | 4.57 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 20 | 4.4 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 14 | 4.38 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 6 | 4.35 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 10 | 4.05 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 12 | 4.02 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 18 | 3.83 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 11 | 3.78 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 5 | 3.73 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 18 | 3.72 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 1 | 3.67 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 17 | 3.66 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 7 | 3.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 17 | 3.6 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 7 | 3.58 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 4 | 3.55 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 19 | 3.54 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 8 | 3.49 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 2 | 3.46 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 2 | 3.46 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 9 | 3.44 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 3 | 3.38 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 4 | 3.36 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 15 | 3.24 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 9 | 3.21 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 15 | 3.18 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 3 | 3.15 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 9 | 3.15 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG11 | 9 | 2.99 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 18 | 2.86 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 8 | 2.85 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 6 | 2.81 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 20 | 2.79 |
| (2,1635) | 1:73:A:LYS:HE3 | 1:33:A:PRO:HB2 | 13 | 2.77 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 1 | 2.71 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG11 | 8 | 2.7 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 3 | 2.66 |
| (4,186) | 1:175:A:PHE:H | 2:201:A:NAD:H2A | 3 | 2.65 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 7 | 2.64 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 7 | 2.59 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG11 | 14 | 2.56 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 10 | 2.53 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 1 | 2.49 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 6 | 2.49 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 17 | 2.44 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 7 | 2.43 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 18 | 2.42 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD13 | 18 | 2.42 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 10 | 2.42 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 15 | 2.41 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG11 | 12 | 2.41 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD13 | 6 | 2.4 |
| (2,1527) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 10 | 2.4 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 5 | 2.39 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 13 | 2.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 8 | 2.37 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD13 | 10 | 2.37 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 11 | 2.37 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 6 | 2.37 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 20 | 2.36 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 3 | 2.36 |
| (4,274) | 1:124:A:LEU:HD22 | 1:159:A:TYR:HE1 | 1 | 2.34 |
| (2,1527) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 1 | 2.34 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 15 | 2.34 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 19 | 2.34 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 9 | 2.33 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 18 | 2.33 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 15 | 2.32 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 14 | 2.32 |
| (2,1527) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 4 | 2.32 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 16 | 2.31 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 1 | 2.3 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 10 | 2.3 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 19 | 2.3 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 7 | 2.29 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 19 | 2.29 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 13 | 2.29 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 12 | 2.28 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 19 | 2.28 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 2 | 2.28 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 4 | 2.28 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 5 | 2.28 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 11 | 2.27 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG12 | 18 | 2.27 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 11 | 2.27 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 5 | 2.27 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 7 | 2.27 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 11 | 2.27 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 6 | 2.27 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 13 | 2.26 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 15 | 2.26 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 3 | 2.26 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 15 | 2.26 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 11 | 2.25 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 9 | 2.25 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 9 | 2.25 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 11 | 2.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 20 | 2.25 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 8 | 2.25 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 16 | 2.24 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 17 | 2.24 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 5 | 2.23 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 17 | 2.23 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 7 | 2.22 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 4 | 2.21 |
| (2,1527) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 3 | 2.21 |
| (2,1471) | 1:57:A:VAL:HG23 | 1:57:A:VAL:H | 12 | 2.21 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 16 | 2.21 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 13 | 2.2 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 15 | 2.2 |
| (2,1527) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 9 | 2.2 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 8 | 2.2 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 14 | 2.2 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 6 | 2.2 |
| (4,315) | 1:56:A:ILE:HG21 | 1:6:A:LYS:HA | 6 | 2.19 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 8 | 2.19 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 3 | 2.19 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 19 | 2.18 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 20 | 2.18 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 16 | 2.18 |
| (2,1471) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 6 | 2.18 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 2 | 2.18 |
| (2,1527) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 7 | 2.17 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 16 | 2.17 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 19 | 2.17 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 12 | 2.16 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 20 | 2.16 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 17 | 2.15 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 15 | 2.14 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 18 | 2.14 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 1 | 2.14 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 15 | 2.14 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 2 | 2.14 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 3 | 2.14 |
| (4,315) | 1:56:A:ILE:HG21 | 1:6:A:LYS:HA | 18 | 2.13 |
| (4,274) | 1:124:A:LEU:HD21 | 1:156:A:PHE:HZ | 13 | 2.13 |
| (4,186) | 1:175:A:PHE:H | 2:201:A:NAD:H2A | 6 | 2.13 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 1 | 2.13 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 8 | 2.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 19 | 2.12 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 16 | 2.12 |
| (4,326) | 1:124:A:LEU:HD22 | 1:177:A:LYS:HE2 | 3 | 2.11 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 3 | 2.11 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 15 | 2.11 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 8 | 2.1 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 16 | 2.1 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 10 | 2.09 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 8 | 2.09 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 1 | 2.09 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 18 | 2.08 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 20 | 2.08 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 18 | 2.08 |
| (4,315) | 1:56:A:ILE:HG22 | 1:6:A:LYS:HA | 9 | 2.07 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 15 | 2.07 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG12 | 2 | 2.07 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 20 | 2.07 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 7 | 2.07 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 13 | 2.07 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 20 | 2.07 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 11 | 2.07 |
| (4,326) | 1:124:A:LEU:HD23 | 1:177:A:LYS:HE2 | 10 | 2.06 |
| (4,326) | 1:124:A:LEU:HD21 | 1:177:A:LYS:HE2 | 13 | 2.06 |
| (4,274) | 1:124:A:LEU:HD21 | 1:156:A:PHE:HZ | 4 | 2.06 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 19 | 2.06 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 6 | 2.05 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 14 | 2.05 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG22 | 12 | 2.05 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 13 | 2.05 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 14 | 2.04 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 3 | 2.04 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 17 | 2.04 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 4 | 2.04 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 2 | 2.03 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 17 | 2.03 |
| (4,326) | 1:124:A:LEU:HD22 | 1:177:A:LYS:HE2 | 4 | 2.02 |
| (4,326) | 1:124:A:LEU:HD23 | 1:177:A:LYS:HE2 | 8 | 2.02 |
| (4,326) | 1:124:A:LEU:HD21 | 1:177:A:LYS:HE2 | 18 | 2.02 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 1 | 2.02 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 4 | 2.02 |
| (4,274) | 1:124:A:LEU:HD22 | 1:159:A:TYR:HE1 | 10 | 2.02 |
| (4,274) | 1:124:A:LEU:HD21 | 1:156:A:PHE:HZ | 12 | 2.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 13 | 2.02 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 5 | 2.01 |
| (4,274) | 1:124:A:LEU:HD23 | 1:156:A:PHE:HZ | 8 | 2.01 |
| (2,1803) | 1:56:A:ILE:HG12 | 1:53:A:LEU:HD12 | 2 | 2.01 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 9 | 2.01 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 20 | 2.01 |
| (4,326) | 1:124:A:LEU:HD21 | 1:177:A:LYS:HE2 | 1 | 2.0 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 16 | 2.0 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 17 | 2.0 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 12 | 2.0 |
| (2,1361) | 1:177:A:LYS:HE2 | 1:147:A:ASP:H | 16 | 2.0 |
| (4,326) | 1:124:A:LEU:HD21 | 1:177:A:LYS:HE2 | 12 | 1.99 |
| (4,186) | 1:175:A:PHE:H | 2:201:A:NAD:H2A | 19 | 1.99 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG22 | 2 | 1.99 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 2 | 1.99 |
| (2,1361) | 1:177:A:LYS:HE2 | 1:147:A:ASP:H | 7 | 1.99 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 7 | 1.98 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 14 | 1.98 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 19 | 1.97 |
| (4,186) | 1:175:A:PHE:H | 2:201:A:NAD:H2A | 16 | 1.97 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 7 | 1.97 |
| (4,326) | 1:124:A:LEU:HD23 | 1:177:A:LYS:HE2 | 5 | 1.96 |
| (4,326) | 1:124:A:LEU:HD23 | 1:177:A:LYS:HE2 | 15 | 1.96 |
| (4,326) | 1:124:A:LEU:HD21 | 1:177:A:LYS:HE2 | 17 | 1.96 |
| (4,316) | 1:37:A:LEU:HD21 | 1:8:A:SER:HB2 | 6 | 1.96 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 4 | 1.96 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 10 | 1.96 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 4 | 1.96 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 10 | 1.95 |
| (2,1802) | 1:53:A:LEU:HD13 | 1:74:A:ILE:HG23 | 10 | 1.95 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 8 | 1.95 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 20 | 1.95 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 11 | 1.94 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 4 | 1.94 |
| (2,32) | 1:88:A:TYR:HE1 | 1:159:A:TYR:HD1 | 20 | 1.94 |
| (4,326) | 1:124:A:LEU:HD21 | 1:177:A:LYS:HE2 | 19 | 1.93 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 2 | 1.93 |
| (4,316) | 1:37:A:LEU:HD21 | 1:8:A:SER:HB2 | 13 | 1.92 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG21 | 7 | 1.92 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 5 | 1.91 |
| (4,326) | 1:124:A:LEU:HD23 | 1:177:A:LYS:HE2 | 20 | 1.91 |
| (4,186) | 1:175:A:PHE:H | 2:201:A:NAD:H2A | 2 | 1.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 3 | 1.91 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 14 | 1.91 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 1 | 1.91 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 17 | 1.91 |
| (4,186) | 1:175:A:PHE:H | 2:201:A:NAD:H2A | 5 | 1.9 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 19 | 1.9 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 19 | 1.88 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 8 | 1.88 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 12 | 1.88 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD13 | 18 | 1.87 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 8 | 1.87 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 11 | 1.87 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 3 | 1.87 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 16 | 1.87 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 1 | 1.86 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 15 | 1.85 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 1 | 1.85 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 17 | 1.85 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 12 | 1.85 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 5 | 1.85 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 18 | 1.85 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 14 | 1.84 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 12 | 1.84 |
| (2,1802) | 1:53:A:LEU:HD13 | 1:74:A:ILE:HG23 | 18 | 1.84 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 11 | 1.84 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 3 | 1.83 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 16 | 1.83 |
| (4,441) | 1:56:A:ILE:HD11 | 1:38:A:LEU:HB2 | 7 | 1.82 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 12 | 1.82 |
| (4,316) | 1:37:A:LEU:HD23 | 1:23:A:GLY:HA3 | 5 | 1.82 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 5 | 1.82 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 5 | 1.82 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 7 | 1.81 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 11 | 1.81 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 17 | 1.81 |
| (4,315) | 1:56:A:ILE:HG23 | 1:38:A:LEU:HA | 20 | 1.81 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 11 | 1.81 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD13 | 10 | 1.8 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 13 | 1.79 |
| (4,326) | 1:124:A:LEU:HD22 | 1:163:A:ASN:HB2 | 9 | 1.79 |
| (4,316) | 1:37:A:LEU:HD21 | 1:8:A:SER:HB2 | 9 | 1.79 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 7 | 1.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1361) | 1:177:A:LYS:HE2 | 1:147:A:ASP:H | 9 | 1.79 |
| (2,1174) | 1:101:A:THR:HG21 | 1:144:A:LEU:HD11 | 12 | 1.79 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 4 | 1.78 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD13 | 6 | 1.78 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 20 | 1.78 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 2 | 1.77 |
| (4,292) | 1:122:A:VAL:HG23 | 1:118:A:SER:H | 3 | 1.77 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 9 | 1.77 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 1 | 1.76 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 20 | 1.76 |
| (4,441) | 1:56:A:ILE:HD12 | 1:6:A:LYS:HB3 | 13 | 1.75 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 18 | 1.75 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 16 | 1.75 |
| (4,326) | 1:124:A:LEU:HD21 | 1:177:A:LYS:HE2 | 6 | 1.75 |
| (4,315) | 1:56:A:ILE:HG22 | 1:38:A:LEU:HA | 14 | 1.75 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG21 | 19 | 1.75 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 13 | 1.75 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 16 | 1.75 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 8 | 1.75 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 8 | 1.74 |
| (4,274) | 1:124:A:LEU:HD23 | 1:156:A:PHE:HZ | 6 | 1.74 |
| (4,186) | 1:175:A:PHE:H | 2:201:A:NAD:H2A | 18 | 1.74 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 9 | 1.73 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 18 | 1.73 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 17 | 1.73 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 2 | 1.73 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 17 | 1.72 |
| (2,1802) | 1:53:A:LEU:HD13 | 1:74:A:ILE:HG23 | 6 | 1.72 |
| (4,441) | 1:56:A:ILE:HD11 | 1:38:A:LEU:HB2 | 6 | 1.71 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 13 | 1.71 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 3 | 1.7 |
| (4,441) | 1:56:A:ILE:HD12 | 1:6:A:LYS:HB3 | 16 | 1.69 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 15 | 1.69 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG12 | 15 | 1.69 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 13 | 1.69 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 13 | 1.69 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 14 | 1.68 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 5 | 1.68 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 4 | 1.68 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 10 | 1.67 |
| (4,435) | 1:24:A:LEU:HB3 | 1:53:A:LEU:HD12 | 19 | 1.67 |
| (4,414) | 1:133:A:LYS:HB2 | 1:128:A:ILE:HG21 | 5 | 1.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 3 | 1.67 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 8 | 1.67 |
| (2,1217) | 1:177:A:LYS:HE2 | 1:177:A:LYS:HB2 | 14 | 1.67 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 9 | 1.67 |
| (4,274) | 1:124:A:LEU:HD22 | 1:159:A:TYR:HE1 | 15 | 1.66 |
| (4,274) | 1:124:A:LEU:HD23 | 1:159:A:TYR:HE1 | 19 | 1.66 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 17 | 1.66 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 15 | 1.65 |
| (2,3498) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 10 | 1.65 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 19 | 1.64 |
| (4,441) | 1:56:A:ILE:HD13 | 1:6:A:LYS:HB3 | 17 | 1.63 |
| (4,415) | 1:19:A:PRO:HB2 | 1:36:A:GLU:HG2 | 3 | 1.63 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 18 | 1.63 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 15 | 1.63 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 4 | 1.63 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 5 | 1.63 |
| (4,441) | 1:56:A:ILE:HD11 | 1:38:A:LEU:HB2 | 9 | 1.62 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 16 | 1.62 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 20 | 1.62 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 6 | 1.62 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 6 | 1.62 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 10 | 1.61 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 5 | 1.61 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 5 | 1.61 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 2 | 1.61 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 3 | 1.61 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 9 | 1.6 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 11 | 1.6 |
| (2,3498) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 1 | 1.6 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 17 | 1.6 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 14 | 1.6 |
| (4,326) | 1:124:A:LEU:HD23 | 1:163:A:ASN:HB2 | 14 | 1.59 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 11 | 1.59 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 15 | 1.59 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 19 | 1.59 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 17 | 1.59 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 12 | 1.59 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 20 | 1.59 |
| (4,292) | 1:122:A:VAL:HG22 | 1:118:A:SER:H | 2 | 1.58 |
| (2,3498) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 4 | 1.58 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 7 | 1.58 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 11 | 1.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,415) | 1:19:A:PRO:HB2 | 1:33:A:PRO:HG2 | 13 | 1.57 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 1 | 1.57 |
| (4,441) | 1:56:A:ILE:HD11 | 1:38:A:LEU:HB2 | 1 | 1.56 |
| (4,326) | 1:124:A:LEU:HD22 | 1:163:A:ASN:HB2 | 16 | 1.56 |
| (4,320) | 1:151:A:MET:HE2 | 1:147:A:ASP:HB2 | 5 | 1.56 |
| (4,316) | 1:37:A:LEU:HD22 | 1:8:A:SER:HB2 | 3 | 1.56 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 19 | 1.56 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 20 | 1.56 |
| (4,326) | 1:124:A:LEU:HD23 | 1:163:A:ASN:HB2 | 11 | 1.55 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 16 | 1.55 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 2 | 1.54 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 17 | 1.54 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 12 | 1.54 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 7 | 1.54 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 2 | 1.54 |
| (2,3454) | 1:168:A:ILE:HD13 | 1:149:A:LYS:H | 12 | 1.53 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 20 | 1.53 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 3 | 1.53 |
| (2,1291) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 2 | 1.53 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 13 | 1.53 |
| (4,415) | 1:19:A:PRO:HB3 | 1:33:A:PRO:HG2 | 4 | 1.52 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 10 | 1.52 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 11 | 1.52 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 14 | 1.52 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 19 | 1.52 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 15 | 1.51 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB2 | 17 | 1.51 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 12 | 1.51 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 2 | 1.51 |
| (4,274) | 1:124:A:LEU:HD23 | 1:159:A:TYR:HE1 | 16 | 1.5 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 17 | 1.5 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 3 | 1.5 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 4 | 1.5 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 11 | 1.5 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 5 | 1.5 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 18 | 1.49 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 8 | 1.49 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 10 | 1.49 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 14 | 1.49 |
| (4,326) | 1:124:A:LEU:HD21 | 1:163:A:ASN:HB2 | 7 | 1.48 |
| (4,320) | 1:151:A:MET:HE2 | 1:147:A:ASP:HB2 | 1 | 1.48 |
| (4,274) | 1:124:A:LEU:HD22 | 1:156:A:PHE:HZ | 5 | 1.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 5 | 1.48 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 13 | 1.48 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 15 | 1.48 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 1 | 1.48 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 16 | 1.48 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 12 | 1.48 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 3 | 1.48 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 9 | 1.48 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 12 | 1.48 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 2 | 1.47 |
| (4,326) | 1:124:A:LEU:HD22 | 1:163:A:ASN:HB2 | 2 | 1.47 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 3 | 1.47 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 13 | 1.47 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 12 | 1.47 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 2 | 1.47 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 6 | 1.47 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 7 | 1.47 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 18 | 1.47 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 14 | 1.47 |
| (4,441) | 1:56:A:ILE:HD12 | 1:38:A:LEU:HB2 | 5 | 1.46 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 10 | 1.46 |
| (2,3498) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 3 | 1.46 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 16 | 1.46 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 14 | 1.46 |
| (2,1421) | 1:21:A:LEU:HD21 | 1:10:A:PHE:HE1 | 11 | 1.46 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 13 | 1.46 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 14 | 1.46 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 20 | 1.46 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD12 | 11 | 1.46 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 15 | 1.46 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 20 | 1.46 |
| (4,441) | 1:56:A:ILE:HD11 | 1:38:A:LEU:HB2 | 8 | 1.45 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 20 | 1.45 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 20 | 1.45 |
| (4,274) | 1:124:A:LEU:HD21 | 1:156:A:PHE:HZ | 3 | 1.45 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 5 | 1.45 |
| (2,3498) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 9 | 1.45 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 4 | 1.45 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 7 | 1.45 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 4 | 1.45 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 8 | 1.45 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 19 | 1.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 8 | 1.45 |
| (2,1421) | 1:21:A:LEU:HD21 | 1:10:A:PHE:HE1 | 4 | 1.45 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 9 | 1.45 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 4 | 1.45 |
| (4,350) | 1:42:A:LYS:HE3 | 1:44:A:LYS:HG2 | 12 | 1.44 |
| (2,1802) | 1:53:A:LEU:HD12 | 1:74:A:ILE:HG23 | 5 | 1.44 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 20 | 1.44 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 2 | 1.44 |
| (2,1421) | 1:21:A:LEU:HD21 | 1:10:A:PHE:HE1 | 6 | 1.44 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 7 | 1.44 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 15 | 1.44 |
| (4,441) | 1:56:A:ILE:HD11 | 1:6:A:LYS:HB3 | 11 | 1.43 |
| (4,441) | 1:56:A:ILE:HD12 | 1:38:A:LEU:HB2 | 12 | 1.43 |
| (4,274) | 1:124:A:LEU:HD21 | 1:159:A:TYR:HE1 | 14 | 1.43 |
| (4,274) | 1:124:A:LEU:HD21 | 1:156:A:PHE:HZ | 18 | 1.43 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 16 | 1.43 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 2 | 1.43 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 12 | 1.43 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 6 | 1.43 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 18 | 1.43 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 17 | 1.43 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 19 | 1.43 |
| (2,1291) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 15 | 1.43 |
| (4,316) | 1:37:A:LEU:HD21 | 1:8:A:SER:HB2 | 20 | 1.42 |
| (2,3498) | 1:38:A:LEU:HD22 | 1:47:A:GLY:HA2 | 7 | 1.42 |
| (2,3454) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 9 | 1.42 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 16 | 1.42 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 7 | 1.42 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 18 | 1.42 |
| (4,292) | 1:122:A:VAL:HG22 | 1:118:A:SER:H | 13 | 1.41 |
| (4,202) | 1:173:A:ALA:HA | 1:145:A:SER:HB2 | 4 | 1.41 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 1 | 1.41 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 6 | 1.41 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 8 | 1.41 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 1 | 1.41 |
| (2,1530) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 3 | 1.41 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 18 | 1.41 |
| (2,1421) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 10 | 1.41 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 3 | 1.41 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB1 | 9 | 1.4 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 12 | 1.4 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 1 | 1.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 8 | 1.4 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 18 | 1.4 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 3 | 1.4 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 20 | 1.4 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 16 | 1.4 |
| (2,1492) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 11 | 1.4 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 6 | 1.4 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 11 | 1.4 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 18 | 1.4 |
| (4,274) | 1:124:A:LEU:HD22 | 1:159:A:TYR:HE1 | 20 | 1.39 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD3 | 2 | 1.39 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 7 | 1.39 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 2 | 1.39 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 14 | 1.39 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 7 | 1.39 |
| (2,1530) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 2 | 1.39 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 11 | 1.39 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 12 | 1.39 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 10 | 1.39 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 14 | 1.38 |
| (2,3454) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 19 | 1.38 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 9 | 1.38 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 10 | 1.38 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 19 | 1.38 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 1 | 1.38 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 3 | 1.38 |
| (4,415) | 1:19:A:PRO:HB2 | 1:33:A:PRO:HG2 | 2 | 1.37 |
| (4,184) | 1:105:A:ASN:H | 1:136:A:MET:H | 17 | 1.37 |
| (2,3830) | 1:97:A:LEU:HD22 | 1:95:A:ALA:HB2 | 4 | 1.37 |
| (2,3830) | 1:97:A:LEU:HD23 | 1:95:A:ALA:HB2 | 5 | 1.37 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 15 | 1.37 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG22 | 16 | 1.37 |
| (2,1738) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 17 | 1.37 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 14 | 1.37 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 14 | 1.37 |
| (2,1530) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 19 | 1.37 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 20 | 1.37 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 17 | 1.37 |
| (2,817) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 1 | 1.37 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 18 | 1.36 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 8 | 1.36 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 9 | 1.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 13 | 1.36 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 17 | 1.36 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 5 | 1.36 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 7 | 1.36 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 11 | 1.36 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 1 | 1.35 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 8 | 1.35 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 7 | 1.35 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 14 | 1.35 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 19 | 1.35 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 15 | 1.35 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 1 | 1.35 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 13 | 1.34 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 8 | 1.34 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 13 | 1.34 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 2 | 1.34 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 11 | 1.34 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 20 | 1.34 |
| (2,1421) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 8 | 1.34 |
| (2,1236) | 1:151:A:MET:HE2 | 1:156:A:PHE:HZ | 9 | 1.34 |
| (4,184) | 1:105:A:ASN:H | 1:136:A:MET:H | 11 | 1.33 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD3 | 18 | 1.33 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 5 | 1.33 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 12 | 1.33 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 18 | 1.33 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD21 | 6 | 1.33 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 9 | 1.33 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 17 | 1.33 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 4 | 1.33 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 12 | 1.33 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 14 | 1.32 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 8 | 1.32 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 10 | 1.32 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 4 | 1.32 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 6 | 1.32 |
| (2,1530) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 10 | 1.32 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 20 | 1.32 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 8 | 1.32 |
| (4,274) | 1:124:A:LEU:HD23 | 1:159:A:TYR:HE1 | 2 | 1.31 |
| (4,202) | 1:173:A:ALA:HA | 1:145:A:SER:HB2 | 19 | 1.31 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 20 | 1.31 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 4 | 1.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 19 | 1.31 |
| (2,1530) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 5 | 1.31 |
| (2,1487) | 1:168:A:ILE:HD13 | 1:149:A:LYS:H | 12 | 1.31 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 20 | 1.31 |
| (4,441) | 1:56:A:ILE:HD11 | 1:6:A:LYS:HB3 | 4 | 1.3 |
| (4,441) | 1:56:A:ILE:HD13 | 1:38:A:LEU:HB2 | 14 | 1.3 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 6 | 1.3 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD3 | 13 | 1.3 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 15 | 1.3 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 17 | 1.3 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 11 | 1.3 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 18 | 1.3 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 8 | 1.3 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 13 | 1.3 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 16 | 1.3 |
| (2,1492) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 5 | 1.3 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 14 | 1.3 |
| (4,292) | 1:122:A:VAL:HG22 | 1:118:A:SER:H | 4 | 1.29 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 8 | 1.29 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 6 | 1.29 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 17 | 1.29 |
| (2,1856) | 1:22:A:ILE:HD12 | 1:14:A:VAL:HG23 | 1 | 1.29 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 8 | 1.29 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 9 | 1.29 |
| (2,1260) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HG11 | 8 | 1.29 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 9 | 1.28 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 18 | 1.28 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 19 | 1.28 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 14 | 1.28 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 3 | 1.28 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB3 | 19 | 1.28 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 14 | 1.28 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 18 | 1.28 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 15 | 1.28 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 3 | 1.28 |
| (2,1291) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 6 | 1.28 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 17 | 1.28 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 4 | 1.28 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 15 | 1.28 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 16 | 1.28 |
| (4,440) | 1:15:A:LEU:HD22 | 1:13:A:LEU:HB2 | 20 | 1.27 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 11 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 12 | 1.27 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 11 | 1.27 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 1 | 1.27 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 20 | 1.27 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 13 | 1.27 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD12 | 2 | 1.27 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 6 | 1.27 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 10 | 1.27 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 18 | 1.27 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 4 | 1.27 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 13 | 1.26 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 12 | 1.26 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 3 | 1.26 |
| (2,3265) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 2 | 1.26 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD21 | 11 | 1.26 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 14 | 1.26 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 13 | 1.26 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 15 | 1.26 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 12 | 1.26 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 7 | 1.26 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 3 | 1.26 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 5 | 1.26 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 6 | 1.26 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 20 | 1.26 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 15 | 1.25 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB1 | 9 | 1.25 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 12 | 1.25 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 10 | 1.25 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 10 | 1.25 |
| (2,1291) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 20 | 1.25 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 7 | 1.25 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 8 | 1.25 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 10 | 1.25 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 17 | 1.25 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 19 | 1.25 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 13 | 1.24 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 13 | 1.24 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 2 | 1.24 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 10 | 1.24 |
| (2,1843) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HB3 | 14 | 1.24 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 13 | 1.24 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 19 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 4 | 1.24 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 16 | 1.24 |
| (2,1361) | 1:177:A:LYS:HE2 | 1:147:A:ASP:H | 11 | 1.24 |
| (2,1361) | 1:177:A:LYS:HE2 | 1:147:A:ASP:H | 14 | 1.24 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 5 | 1.23 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 3 | 1.23 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 14 | 1.23 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG23 | 3 | 1.23 |
| (2,1843) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HB3 | 15 | 1.23 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 2 | 1.23 |
| (2,1452) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 6 | 1.23 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 4 | 1.23 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 1 | 1.23 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 4 | 1.22 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 19 | 1.22 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 10 | 1.22 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 1 | 1.22 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 3 | 1.22 |
| (2,3830) | 1:97:A:LEU:HD22 | 1:95:A:ALA:HB1 | 10 | 1.22 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 13 | 1.22 |
| (2,1868) | 1:97:A:LEU:HD22 | 1:95:A:ALA:HB2 | 4 | 1.22 |
| (2,1868) | 1:97:A:LEU:HD23 | 1:95:A:ALA:HB2 | 5 | 1.22 |
| (2,1843) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HB3 | 5 | 1.22 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 6 | 1.22 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 5 | 1.22 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 12 | 1.22 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 3 | 1.22 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 15 | 1.22 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 9 | 1.22 |
| (2,1452) | 1:38:A:LEU:HD11 | 1:38:A:LEU:H | 19 | 1.22 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 20 | 1.22 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 13 | 1.22 |
| (4,274) | 1:124:A:LEU:HD21 | 1:159:A:TYR:HE1 | 7 | 1.21 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB3 | 7 | 1.21 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 4 | 1.21 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 7 | 1.21 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 20 | 1.21 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 2 | 1.21 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 8 | 1.21 |
| (2,1843) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HB3 | 9 | 1.21 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 12 | 1.21 |
| (2,1806) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HB2 | 12 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 1 | 1.21 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 12 | 1.21 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 17 | 1.21 |
| (2,1452) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 1 | 1.21 |
| (2,1452) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 4 | 1.21 |
| (2,1452) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 14 | 1.21 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 15 | 1.21 |
| (2,1291) | 1:84:A:VAL:HG13 | 1:84:A:VAL:H | 1 | 1.21 |
| (4,436) | 1:178:A:VAL:HG13 | 1:110:A:LEU:HB3 | 3 | 1.2 |
| (4,103) | 1:114:A:ILE:H | 1:123:A:HIS:HA | 6 | 1.2 |
| (4,103) | 1:114:A:ILE:H | 1:123:A:HIS:HA | 16 | 1.2 |
| (4,7) | 1:65:A:PHE:HZ | 1:37:A:LEU:HD21 | 5 | 1.2 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 16 | 1.2 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 2 | 1.2 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 12 | 1.2 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 13 | 1.2 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 13 | 1.2 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 16 | 1.2 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 19 | 1.2 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 19 | 1.2 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD21 | 4 | 1.2 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 9 | 1.2 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 14 | 1.2 |
| (2,1487) | 1:168:A:ILE:HD12 | 1:149:A:LYS:H | 9 | 1.2 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 1 | 1.2 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 3 | 1.2 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 10 | 1.2 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 4 | 1.2 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 11 | 1.2 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 18 | 1.2 |
| (4,184) | 1:105:A:ASN:H | 1:136:A:MET:H | 16 | 1.19 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 17 | 1.19 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 18 | 1.19 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 17 | 1.19 |
| (2,1492) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 2 | 1.19 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 2 | 1.19 |
| (2,1452) | 1:38:A:LEU:HD11 | 1:38:A:LEU:H | 7 | 1.19 |
| (2,1452) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 11 | 1.19 |
| (2,1452) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 17 | 1.19 |
| (2,1452) | 1:38:A:LEU:HD11 | 1:38:A:LEU:H | 18 | 1.19 |
| (2,1260) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HG11 | 15 | 1.19 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 13 | 1.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 2 | 1.19 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 7 | 1.18 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 8 | 1.18 |
| (4,320) | 1:151:A:MET:HE1 | 1:147:A:ASP:HB2 | 19 | 1.18 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 9 | 1.18 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 18 | 1.18 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD13 | 14 | 1.18 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 15 | 1.18 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 8 | 1.18 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 5 | 1.18 |
| (2,1260) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HG11 | 10 | 1.18 |
| (2,1217) | 1:177:A:LYS:HE2 | 1:177:A:LYS:HB2 | 7 | 1.18 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 5 | 1.18 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 1 | 1.18 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 13 | 1.17 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 3 | 1.17 |
| (2,3830) | 1:97:A:LEU:HD23 | 1:95:A:ALA:HB2 | 6 | 1.17 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 1 | 1.17 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 6 | 1.17 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 18 | 1.17 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 11 | 1.17 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 18 | 1.17 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 18 | 1.17 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 14 | 1.17 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 20 | 1.17 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 7 | 1.17 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 8 | 1.17 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 13 | 1.17 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 1 | 1.17 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 16 | 1.17 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 9 | 1.17 |
| (2,336) | 1:176:A:ILE:H | 1:176:A:ILE:HG12 | 14 | 1.17 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 12 | 1.17 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 19 | 1.16 |
| (4,415) | 1:19:A:PRO:HB2 | 1:36:A:GLU:HG2 | 7 | 1.16 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 1 | 1.16 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 7 | 1.16 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 15 | 1.16 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 16 | 1.16 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 8 | 1.16 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 7 | 1.16 |
| (2,3265) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 15 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 3 | 1.16 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 5 | 1.16 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 6 | 1.16 |
| (2,1806) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HB2 | 8 | 1.16 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 16 | 1.16 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 19 | 1.16 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 3 | 1.16 |
| (2,1452) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 12 | 1.16 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG12 | 7 | 1.16 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 18 | 1.16 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG12 | 19 | 1.16 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 10 | 1.16 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 2 | 1.15 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 3 | 1.15 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 4 | 1.15 |
| (4,378) | 1:24:A:LEU:HA | 1:15:A:LEU:HB2 | 11 | 1.15 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 13 | 1.15 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 8 | 1.15 |
| (4,202) | 1:173:A:ALA:HA | 1:145:A:SER:HB2 | 5 | 1.15 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 10 | 1.15 |
| (2,3807) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HB3 | 14 | 1.15 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 9 | 1.15 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 10 | 1.15 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 19 | 1.15 |
| (2,3501) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 3 | 1.15 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 11 | 1.15 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 1 | 1.15 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 3 | 1.15 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 7 | 1.15 |
| (2,1806) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HB2 | 11 | 1.15 |
| (2,1806) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HB2 | 13 | 1.15 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 14 | 1.15 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 10 | 1.15 |
| (2,1561) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 20 | 1.15 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 18 | 1.15 |
| (2,1487) | 1:168:A:ILE:HD11 | 1:149:A:LYS:H | 19 | 1.15 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 4 | 1.15 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 20 | 1.15 |
| (4,436) | 1:178:A:VAL:HG13 | 1:110:A:LEU:HB3 | 17 | 1.14 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 15 | 1.14 |
| (4,274) | 1:124:A:LEU:HD21 | 1:159:A:TYR:HE1 | 11 | 1.14 |
| (2,3807) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HB3 | 5 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3807) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HB3 | 15 | 1.14 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 15 | 1.14 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG23 | 17 | 1.14 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 11 | 1.14 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 16 | 1.14 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 8 | 1.14 |
| (2,1856) | 1:22:A:ILE:HD13 | 1:14:A:VAL:HG21 | 20 | 1.14 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 5 | 1.14 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 4 | 1.14 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG21 | 5 | 1.14 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 15 | 1.14 |
| (2,1561) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 5 | 1.14 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 13 | 1.14 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 16 | 1.14 |
| (2,1549) | 1:37:A:LEU:HD12 | 1:41:A:MET:HG2 | 1 | 1.14 |
| (2,1452) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 16 | 1.14 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 18 | 1.14 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 6 | 1.14 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 19 | 1.14 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 6 | 1.14 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD23 | 2 | 1.13 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 3 | 1.13 |
| (4,440) | 1:15:A:LEU:HD23 | 1:74:A:ILE:HB | 4 | 1.13 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 18 | 1.13 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 12 | 1.13 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 6 | 1.13 |
| (2,3704) | 1:7:A:VAL:HA | 1:22:A:ILE:HG22 | 16 | 1.13 |
| (2,3501) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 2 | 1.13 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 12 | 1.13 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB3 | 19 | 1.13 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 18 | 1.13 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 13 | 1.13 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 4 | 1.13 |
| (4,313) | 1:96:A:VAL:HG13 | 1:145:A:SER:HA | 5 | 1.12 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 2 | 1.12 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 8 | 1.12 |
| (2,3807) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HB3 | 9 | 1.12 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 12 | 1.12 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 13 | 1.12 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 1 | 1.12 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG22 | 20 | 1.12 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD13 | 10 | 1.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1559) | 1:21:A:LEU:HD21 | 1:41:A:MET:HB2 | 6 | 1.12 |
| (2,1549) | 1:37:A:LEU:HD12 | 1:41:A:MET:HG2 | 3 | 1.12 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 7 | 1.12 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 5 | 1.12 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 8 | 1.12 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 17 | 1.12 |
| (4,103) | 1:114:A:ILE:H | 1:123:A:HIS:HA | 8 | 1.11 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD23 | 6 | 1.11 |
| (4,7) | 1:65:A:PHE:HZ | 1:37:A:LEU:HD23 | 12 | 1.11 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 16 | 1.11 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 19 | 1.11 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 10 | 1.11 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 8 | 1.11 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 13 | 1.11 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 14 | 1.11 |
| (2,3501) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 19 | 1.11 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 20 | 1.11 |
| (2,1806) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HB2 | 2 | 1.11 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 15 | 1.11 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 20 | 1.11 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 3 | 1.11 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 5 | 1.11 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 10 | 1.11 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 11 | 1.11 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 13 | 1.11 |
| (4,436) | 1:178:A:VAL:HG13 | 1:110:A:LEU:HB3 | 20 | 1.1 |
| (4,353) | 1:84:A:VAL:HB | 1:87:A:GLY:HA2 | 20 | 1.1 |
| (4,186) | 1:133:A:LYS:H | 2:201:A:NAD:H5N | 4 | 1.1 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 20 | 1.1 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 18 | 1.1 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 9 | 1.1 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 17 | 1.1 |
| (2,1851) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 17 | 1.1 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD11 | 13 | 1.1 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 9 | 1.1 |
| (2,1806) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 10 | 1.1 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 12 | 1.1 |
| (2,1559) | 1:21:A:LEU:HD21 | 1:41:A:MET:HB2 | 11 | 1.1 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 2 | 1.1 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 9 | 1.1 |
| (2,1500) | 1:11:A:LEU:HD12 | 1:38:A:LEU:HA | 6 | 1.1 |
| (2,1492) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 18 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 19 | 1.1 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 8 | 1.1 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 16 | 1.1 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 17 | 1.09 |
| (4,36) | 1:76:A:ALA:H | 1:57:A:VAL:HG23 | 15 | 1.09 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 9 | 1.09 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 7 | 1.09 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 14 | 1.09 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 15 | 1.09 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD11 | 7 | 1.09 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 2 | 1.09 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 11 | 1.09 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 1 | 1.09 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 3 | 1.09 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 9 | 1.09 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 18 | 1.09 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 12 | 1.08 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 20 | 1.08 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 3 | 1.08 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 4 | 1.08 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 12 | 1.08 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 19 | 1.08 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG21 | 5 | 1.08 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 10 | 1.08 |
| (2,3527) | 1:84:A:VAL:HG21 | 1:85:A:ASP:HB2 | 2 | 1.08 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 14 | 1.08 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 18 | 1.08 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 4 | 1.08 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 12 | 1.08 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 13 | 1.08 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG12 | 14 | 1.08 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 8 | 1.08 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 11 | 1.07 |
| (4,436) | 1:178:A:VAL:HG13 | 1:110:A:LEU:HB3 | 1 | 1.07 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 5 | 1.07 |
| (4,378) | 1:24:A:LEU:HA | 1:15:A:LEU:HB2 | 7 | 1.07 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG2 | 20 | 1.07 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 6 | 1.07 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 4 | 1.07 |
| (2,1868) | 1:97:A:LEU:HD22 | 1:95:A:ALA:HB1 | 10 | 1.07 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 13 | 1.07 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 2 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 15 | 1.07 |
| (2,1549) | 1:37:A:LEU:HD11 | 1:41:A:MET:HG2 | 16 | 1.07 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 2 | 1.07 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 6 | 1.07 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 14 | 1.07 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 17 | 1.07 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 16 | 1.07 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD12 | 20 | 1.07 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD22 | 2 | 1.06 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 9 | 1.06 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 10 | 1.06 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 8 | 1.06 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 18 | 1.06 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 11 | 1.06 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD21 | 6 | 1.06 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 10 | 1.06 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 9 | 1.06 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 6 | 1.06 |
| (2,3501) | 1:178:A:VAL:HG22 | 1:109:A:ILE:HA | 10 | 1.06 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB3 | 7 | 1.06 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 15 | 1.06 |
| (2,1492) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 10 | 1.06 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 11 | 1.06 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 14 | 1.06 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 15 | 1.06 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 19 | 1.06 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 10 | 1.06 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 7 | 1.05 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 2 | 1.05 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 15 | 1.05 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 12 | 1.05 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 14 | 1.05 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 11 | 1.05 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 2 | 1.05 |
| (2,3847) | 1:41:A:MET:HE1 | 1:46:A:HIS:HA | 7 | 1.05 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 2 | 1.05 |
| (2,3501) | 1:178:A:VAL:HG21 | 1:109:A:ILE:HA | 5 | 1.05 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 16 | 1.05 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 20 | 1.05 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 18 | 1.05 |
| (2,1559) | 1:21:A:LEU:HD21 | 1:41:A:MET:HB2 | 4 | 1.05 |
| (2,1559) | 1:21:A:LEU:HD22 | 1:41:A:MET:HB2 | 9 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1549) | 1:37:A:LEU:HD11 | 1:41:A:MET:HG2 | 11 | 1.05 |
| (2,1549) | 1:37:A:LEU:HD11 | 1:41:A:MET:HG2 | 15 | 1.05 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 7 | 1.05 |
| (2,1492) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 15 | 1.05 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 10 | 1.05 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 16 | 1.05 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 17 | 1.05 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 6 | 1.05 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 9 | 1.05 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 2 | 1.05 |
| (4,436) | 1:178:A:VAL:HG13 | 1:110:A:LEU:HB3 | 4 | 1.04 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 10 | 1.04 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD13 | 16 | 1.04 |
| (4,329) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HA | 19 | 1.04 |
| (4,184) | 1:105:A:ASN:H | 1:136:A:MET:H | 6 | 1.04 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 10 | 1.04 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 11 | 1.04 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 15 | 1.04 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 17 | 1.04 |
| (2,3500) | 1:144:A:LEU:HD23 | 1:145:A:SER:HB2 | 6 | 1.04 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 17 | 1.04 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 17 | 1.04 |
| (2,1851) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD11 | 12 | 1.04 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD11 | 1 | 1.04 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 1 | 1.04 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 4 | 1.04 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 5 | 1.04 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 20 | 1.04 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 4 | 1.04 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 10 | 1.04 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 1 | 1.04 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 7 | 1.04 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 6 | 1.04 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 5 | 1.04 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD13 | 6 | 1.03 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD12 | 14 | 1.03 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 15 | 1.03 |
| (2,3847) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 8 | 1.03 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 8 | 1.03 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 17 | 1.03 |
| (2,1807) | 1:151:A:MET:HE3 | 1:174:A:GLU:HG2 | 14 | 1.03 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 6 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1500) | 1:11:A:LEU:HD12 | 1:38:A:LEU:HA | 10 | 1.03 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 18 | 1.03 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 11 | 1.03 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 4 | 1.03 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 14 | 1.03 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 18 | 1.03 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 6 | 1.03 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 16 | 1.03 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 1 | 1.03 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 2 | 1.03 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 12 | 1.03 |
| (4,415) | 1:19:A:PRO:HB2 | 1:36:A:GLU:HG2 | 8 | 1.02 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD13 | 11 | 1.02 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 2 | 1.02 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 13 | 1.02 |
| (2,3847) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 6 | 1.02 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 9 | 1.02 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 18 | 1.02 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 3 | 1.02 |
| (2,1868) | 1:97:A:LEU:HD23 | 1:95:A:ALA:HB2 | 6 | 1.02 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 17 | 1.02 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 9 | 1.02 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 13 | 1.02 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 10 | 1.02 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 13 | 1.02 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 17 | 1.02 |
| (2,1441) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 5 | 1.02 |
| (2,1441) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 20 | 1.02 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 1 | 1.02 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 2 | 1.02 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 11 | 1.02 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 19 | 1.02 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 20 | 1.02 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 7 | 1.02 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 8 | 1.02 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 11 | 1.02 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 12 | 1.02 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 14 | 1.02 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 18 | 1.02 |
| (4,440) | 1:15:A:LEU:HD23 | 1:13:A:LEU:HB2 | 5 | 1.01 |
| (4,436) | 1:178:A:VAL:HG11 | 1:110:A:LEU:HB3 | 7 | 1.01 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 2 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD21 | 5 | 1.01 |
| (2,3830) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB1 | 1 | 1.01 |
| (2,3265) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 6 | 1.01 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 15 | 1.01 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG23 | 17 | 1.01 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 3 | 1.01 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 8 | 1.01 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 8 | 1.01 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 3 | 1.01 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 9 | 1.01 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 12 | 1.01 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 14 | 1.01 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 2 | 1.01 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 10 | 1.01 |
| (2,1549) | 1:37:A:LEU:HD11 | 1:41:A:MET:HG2 | 12 | 1.01 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 5 | 1.01 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 3 | 1.01 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 8 | 1.01 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 17 | 1.01 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 4 | 1.01 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 13 | 1.01 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 17 | 1.01 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 8 | 1.01 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 3 | 1.0 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD21 | 11 | 1.0 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 15 | 1.0 |
| (2,1851) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD11 | 4 | 1.0 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 18 | 1.0 |
| (2,1843) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 7 | 1.0 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 10 | 1.0 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 14 | 1.0 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 7 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 2 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 3 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 5 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 7 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 10 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 11 | 1.0 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 12 | 1.0 |
| (2,1217) | 1:177:A:LYS:HE2 | 1:177:A:LYS:HB2 | 16 | 1.0 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 17 | 1.0 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 15 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 2 | 1.0 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 10 | 1.0 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 15 | 1.0 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD21 | 9 | 0.99 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 8 | 0.99 |
| (4,313) | 1:96:A:VAL:HG13 | 1:145:A:SER:HA | 7 | 0.99 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 12 | 0.99 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD13 | 19 | 0.99 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 20 | 0.99 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 9 | 0.99 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD12 | 18 | 0.99 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 18 | 0.99 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 8 | 0.99 |
| (2,1495) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 12 | 0.99 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 2 | 0.99 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 4 | 0.99 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 16 | 0.99 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 19 | 0.99 |
| (2,1291) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 11 | 0.99 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 1 | 0.99 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 2 | 0.99 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 4 | 0.99 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 9 | 0.99 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 9 | 0.99 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 19 | 0.99 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 1 | 0.99 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 2 | 0.99 |
| (2,21) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 7 | 0.99 |
| (4,458) | 1:50:A:MET:HE2 | 1:50:A:MET:HA | 13 | 0.98 |
| (4,320) | 1:151:A:MET:HE3 | 1:147:A:ASP:HB2 | 7 | 0.98 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 8 | 0.98 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 19 | 0.98 |
| (2,3265) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 20 | 0.98 |
| (2,1830) | 1:34:A:VAL:HG12 | 1:50:A:MET:HE1 | 18 | 0.98 |
| (2,1495) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 11 | 0.98 |
| (2,1467) | 1:14:A:VAL:HG13 | 1:10:A:PHE:HD1 | 5 | 0.98 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 1 | 0.98 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 6 | 0.98 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 8 | 0.98 |
| (2,1444) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 9 | 0.98 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 20 | 0.98 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 12 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 12 | 0.98 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 19 | 0.98 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 14 | 0.98 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 10 | 0.97 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 12 | 0.97 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 15 | 0.97 |
| (4,301) | 1:97:A:LEU:HD23 | 1:175:A:PHE:HB2 | 17 | 0.97 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 4 | 0.97 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 20 | 0.97 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 15 | 0.97 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 19 | 0.97 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 13 | 0.97 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 12 | 0.97 |
| (2,3527) | 1:84:A:VAL:HG21 | 1:85:A:ASP:HB2 | 15 | 0.97 |
| (2,1830) | 1:34:A:VAL:HG12 | 1:50:A:MET:HE2 | 1 | 0.97 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 17 | 0.97 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 18 | 0.97 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 16 | 0.97 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 5 | 0.97 |
| (2,1559) | 1:21:A:LEU:HD23 | 1:41:A:MET:HB2 | 19 | 0.97 |
| (2,1554) | 1:38:A:LEU:HD21 | 1:50:A:MET:HG2 | 12 | 0.97 |
| (2,1549) | 1:37:A:LEU:HD13 | 1:41:A:MET:HG2 | 2 | 0.97 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 4 | 0.97 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 8 | 0.97 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 15 | 0.97 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 16 | 0.97 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 6 | 0.97 |
| (2,1444) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 14 | 0.97 |
| (2,1444) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 15 | 0.97 |
| (2,1291) | 1:84:A:VAL:HG13 | 1:84:A:VAL:H | 18 | 0.97 |
| (2,1260) | 1:142:A:VAL:HG21 | 1:178:A:VAL:HG11 | 9 | 0.97 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 7 | 0.97 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 13 | 0.97 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 16 | 0.97 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 7 | 0.97 |
| (2,21) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 13 | 0.97 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD22 | 5 | 0.96 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 6 | 0.96 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD12 | 15 | 0.96 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 6 | 0.96 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 10 | 0.96 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 14 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,378) | 1:24:A:LEU:HA | 1:15:A:LEU:HB2 | 20 | 0.96 |
| (4,313) | 1:143:A:VAL:HG12 | 1:145:A:SER:HA | 13 | 0.96 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 14 | 0.96 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 12 | 0.96 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 2 | 0.96 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 4 | 0.96 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 4 | 0.96 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 8 | 0.96 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 4 | 0.96 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 20 | 0.96 |
| (2,3771) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HB2 | 12 | 0.96 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 2 | 0.96 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 5 | 0.96 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 5 | 0.96 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 6 | 0.96 |
| (2,1742) | 1:110:A:LEU:HD11 | 1:173:A:ALA:HA | 5 | 0.96 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 7 | 0.96 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 12 | 0.96 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 3 | 0.96 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 17 | 0.96 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 13 | 0.96 |
| (2,1495) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 1 | 0.96 |
| (2,1291) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 14 | 0.96 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 18 | 0.96 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 5 | 0.96 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 3 | 0.96 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 6 | 0.96 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 11 | 0.96 |
| (2,339) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 18 | 0.96 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD23 | 8 | 0.95 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD21 | 13 | 0.95 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 5 | 0.95 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 8 | 0.95 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 19 | 0.95 |
| (4,349) | 1:39:A:ALA:HB1 | 1:42:A:LYS:HE2 | 20 | 0.95 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 1 | 0.95 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 20 | 0.95 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 1 | 0.95 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 11 | 0.95 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 12 | 0.95 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 1 | 0.95 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 12 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 14 | 0.95 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 18 | 0.95 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 10 | 0.95 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 11 | 0.95 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 2 | 0.95 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 6 | 0.95 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 15 | 0.95 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 20 | 0.95 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 4 | 0.95 |
| (2,1527) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 12 | 0.95 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 5 | 0.95 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 10 | 0.95 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 9 | 0.95 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 19 | 0.95 |
| (2,1495) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 5 | 0.95 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 11 | 0.95 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 2 | 0.95 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 4 | 0.95 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 9 | 0.95 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 18 | 0.95 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 20 | 0.95 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 18 | 0.95 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG13 | 12 | 0.95 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 14 | 0.94 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD13 | 19 | 0.94 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 11 | 0.94 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 16 | 0.94 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD13 | 14 | 0.94 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 6 | 0.94 |
| (4,292) | 1:122:A:VAL:HG21 | 1:118:A:SER:H | 19 | 0.94 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 11 | 0.94 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 3 | 0.94 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD13 | 8 | 0.94 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 17 | 0.94 |
| (2,3847) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 18 | 0.94 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 17 | 0.94 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD21 | 4 | 0.94 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 3 | 0.94 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 9 | 0.94 |
| (2,3265) | 1:84:A:VAL:HG13 | 1:84:A:VAL:H | 1 | 0.94 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 8 | 0.94 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 13 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 16 | 0.94 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 19 | 0.94 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 11 | 0.94 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 19 | 0.94 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 17 | 0.94 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 9 | 0.94 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 1 | 0.94 |
| (2,816) | 1:53:A:LEU:HD22 | 1:53:A:LEU:H | 6 | 0.94 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 10 | 0.94 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 19 | 0.94 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 10 | 0.94 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 7 | 0.94 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD12 | 5 | 0.93 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD22 | 18 | 0.93 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 7 | 0.93 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 16 | 0.93 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 16 | 0.93 |
| (4,329) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HA | 11 | 0.93 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 1 | 0.93 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD23 | 13 | 0.93 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 19 | 0.93 |
| (4,9) | 1:10:A:PHE:HD1 | 1:7:A:VAL:HG11 | 5 | 0.93 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD22 | 3 | 0.93 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD21 | 13 | 0.93 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 17 | 0.93 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 7 | 0.93 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 18 | 0.93 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG23 | 16 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 3 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD11 | 11 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 13 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 15 | 0.93 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 16 | 0.93 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 10 | 0.93 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 14 | 0.93 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 19 | 0.93 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 18 | 0.93 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 5 | 0.93 |
| (2,1549) | 1:37:A:LEU:HD12 | 1:41:A:MET:HG2 | 9 | 0.93 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 4 | 0.93 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 13 | 0.93 |
| (2,1236) | 1:151:A:MET:HE1 | 1:156:A:PHE:HZ | 17 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 5 | 0.93 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 10 | 0.93 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 14 | 0.93 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 7 | 0.93 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 11 | 0.93 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 5 | 0.93 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 10 | 0.93 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 7 | 0.92 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD13 | 20 | 0.92 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 1 | 0.92 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 3 | 0.92 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 8 | 0.92 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 13 | 0.92 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 18 | 0.92 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 15 | 0.92 |
| (4,300) | 1:97:A:LEU:HD21 | 1:175:A:PHE:HB3 | 9 | 0.92 |
| (4,244) | 1:51:A:GLU:HG2 | 1:67:A:PHE:HD1 | 5 | 0.92 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 19 | 0.92 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 12 | 0.92 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 15 | 0.92 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 14 | 0.92 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 8 | 0.92 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 1 | 0.92 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 5 | 0.92 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD22 | 10 | 0.92 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 18 | 0.92 |
| (2,3847) | 1:41:A:MET:HE3 | 1:46:A:HIS:HA | 20 | 0.92 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD13 | 14 | 0.92 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 3 | 0.92 |
| (2,3807) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HB3 | 7 | 0.92 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 20 | 0.92 |
| (2,3527) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 20 | 0.92 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 4 | 0.92 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 7 | 0.92 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 9 | 0.92 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 12 | 0.92 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 17 | 0.92 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 19 | 0.92 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 11 | 0.92 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD12 | 12 | 0.92 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 17 | 0.92 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 18 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 20 | 0.92 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 4 | 0.92 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 17 | 0.92 |
| (2,1549) | 1:37:A:LEU:HD11 | 1:41:A:MET:HG2 | 4 | 0.92 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 1 | 0.92 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 5 | 0.92 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 17 | 0.92 |
| (2,1468) | 1:22:A:ILE:HG21 | 1:10:A:PHE:HZ | 16 | 0.92 |
| (2,1107) | 1:118:A:SER:H | 2:201:A:NAD:H51A | 1 | 0.92 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 13 | 0.92 |
| (2,816) | 1:53:A:LEU:HD22 | 1:53:A:LEU:H | 16 | 0.92 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 3 | 0.92 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 18 | 0.92 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 19 | 0.92 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD23 | 10 | 0.91 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 4 | 0.91 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 10 | 0.91 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 17 | 0.91 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 19 | 0.91 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 18 | 0.91 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 20 | 0.91 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 13 | 0.91 |
| (4,202) | 1:173:A:ALA:HA | 1:145:A:SER:HB2 | 12 | 0.91 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 15 | 0.91 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 18 | 0.91 |
| (2,3837) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 11 | 0.91 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 5 | 0.91 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 5 | 0.91 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 6 | 0.91 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 16 | 0.91 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 19 | 0.91 |
| (2,3508) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 1 | 0.91 |
| (2,3462) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 12 | 0.91 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 1 | 0.91 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 9 | 0.91 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 18 | 0.91 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 7 | 0.91 |
| (2,1865) | 1:109:A:ILE:HD11 | 1:144:A:LEU:HD11 | 12 | 0.91 |
| (2,1851) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 1 | 0.91 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 6 | 0.91 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 19 | 0.91 |
| (2,1807) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 20 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 10 | 0.91 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 13 | 0.91 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 14 | 0.91 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 16 | 0.91 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 6 | 0.91 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 19 | 0.91 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 20 | 0.91 |
| (2,1495) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 7 | 0.91 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 18 | 0.91 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 18 | 0.91 |
| (2,1291) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 8 | 0.91 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 11 | 0.91 |
| (2,339) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 19 | 0.91 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 13 | 0.91 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 15 | 0.91 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 18 | 0.91 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 4 | 0.91 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 7 | 0.91 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 11 | 0.91 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 12 | 0.91 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 13 | 0.91 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 19 | 0.91 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 15 | 0.91 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 4 | 0.91 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 9 | 0.91 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD22 | 3 | 0.9 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 14 | 0.9 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 15 | 0.9 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 20 | 0.9 |
| (4,292) | 1:122:A:VAL:HG23 | 1:118:A:SER:H | 1 | 0.9 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 3 | 0.9 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 4 | 0.9 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 16 | 0.9 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 19 | 0.9 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 7 | 0.9 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 13 | 0.9 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 3 | 0.9 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 12 | 0.9 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD22 | 2 | 0.9 |
| (2,3837) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 10 | 0.9 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 3 | 0.9 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 7 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3771) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HB2 | 8 | 0.9 |
| (2,3771) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HB2 | 13 | 0.9 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 14 | 0.9 |
| (2,3462) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 11 | 0.9 |
| (2,2266) | 1:153:A:ASP:H | 1:95:A:ALA:HB1 | 5 | 0.9 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 13 | 0.9 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 10 | 0.9 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 14 | 0.9 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 4 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD22 | 2 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD22 | 3 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 7 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 9 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 16 | 0.9 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 18 | 0.9 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 11 | 0.9 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 17 | 0.9 |
| (2,1535) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HE3 | 12 | 0.9 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 9 | 0.9 |
| (2,1495) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 14 | 0.9 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 20 | 0.9 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 16 | 0.9 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 12 | 0.9 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 6 | 0.9 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 8 | 0.9 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 9 | 0.9 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 17 | 0.9 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 8 | 0.9 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 5 | 0.9 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 9 | 0.89 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 18 | 0.89 |
| (4,378) | 1:24:A:LEU:HA | 1:21:A:LEU:HG | 17 | 0.89 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 9 | 0.89 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 7 | 0.89 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 20 | 0.89 |
| (4,204) | 1:173:A:ALA:HB1 | 1:111:A:LYS:HG3 | 2 | 0.89 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 2 | 0.89 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 11 | 0.89 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 10 | 0.89 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 7 | 0.89 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 1 | 0.89 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 14 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 1 | 0.89 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 4 | 0.89 |
| (2,3771) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HB2 | 11 | 0.89 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 7 | 0.89 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 6 | 0.89 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 3 | 0.89 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB2 | 11 | 0.89 |
| (2,1865) | 1:109:A:ILE:HD11 | 1:144:A:LEU:HD13 | 19 | 0.89 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 20 | 0.89 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 10 | 0.89 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 8 | 0.89 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 8 | 0.89 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 17 | 0.89 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 19 | 0.89 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 11 | 0.89 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 1 | 0.89 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 12 | 0.89 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 15 | 0.89 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 8 | 0.89 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 18 | 0.89 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 2 | 0.89 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 7 | 0.89 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 18 | 0.89 |
| (2,1490) | 1:167:A:LEU:HD11 | 1:166:A:TRP:HA | 17 | 0.89 |
| (2,1291) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 10 | 0.89 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 15 | 0.89 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 8 | 0.89 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 1 | 0.89 |
| (2,816) | 1:53:A:LEU:HD21 | 1:53:A:LEU:H | 2 | 0.89 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 2 | 0.89 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 10 | 0.89 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 14 | 0.89 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 15 | 0.89 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 16 | 0.89 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 18 | 0.89 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 12 | 0.89 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD22 | 12 | 0.88 |
| (4,397) | 1:56:A:ILE:HA | 1:54:A:LYS:HB2 | 12 | 0.88 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD13 | 3 | 0.88 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 13 | 0.88 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 7 | 0.88 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 14 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3837) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 5 | 0.88 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 18 | 0.88 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 19 | 0.88 |
| (2,3508) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 3 | 0.88 |
| (2,3421) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 6 | 0.88 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 4 | 0.88 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 11 | 0.88 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 20 | 0.88 |
| (2,1851) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 9 | 0.88 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 1 | 0.88 |
| (2,1845) | 1:176:A:ILE:HB | 1:110:A:LEU:HD11 | 9 | 0.88 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 18 | 0.88 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 6 | 0.88 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 11 | 0.88 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 20 | 0.88 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 3 | 0.88 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 14 | 0.88 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 16 | 0.88 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 13 | 0.88 |
| (2,1291) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 9 | 0.88 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 16 | 0.88 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 3 | 0.88 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 4 | 0.88 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 10 | 0.88 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 13 | 0.88 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 9 | 0.88 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 19 | 0.88 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 11 | 0.88 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD13 | 9 | 0.87 |
| (4,292) | 1:122:A:VAL:HG22 | 1:118:A:SER:H | 10 | 0.87 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 13 | 0.87 |
| (4,103) | 1:114:A:ILE:H | 1:123:A:HIS:HA | 20 | 0.87 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 1 | 0.87 |
| (2,3772) | 1:151:A:MET:HE3 | 1:174:A:GLU:HG2 | 14 | 0.87 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 18 | 0.87 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 17 | 0.87 |
| (2,3462) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 1 | 0.87 |
| (2,3462) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 5 | 0.87 |
| (2,3421) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 1 | 0.87 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 9 | 0.87 |
| (2,3421) | 1:38:A:LEU:HD11 | 1:38:A:LEU:H | 19 | 0.87 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 20 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 8 | 0.87 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 15 | 0.87 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 3 | 0.87 |
| (2,1851) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 7 | 0.87 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 15 | 0.87 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 13 | 0.87 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 12 | 0.87 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 8 | 0.87 |
| (2,1554) | 1:38:A:LEU:HD21 | 1:50:A:MET:HG2 | 3 | 0.87 |
| (2,1529) | 1:144:A:LEU:HD23 | 1:145:A:SER:HB2 | 6 | 0.87 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 12 | 0.87 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 2 | 0.87 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 17 | 0.87 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD23 | 12 | 0.86 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 13 | 0.86 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 14 | 0.86 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 10 | 0.86 |
| (4,320) | 1:151:A:MET:HE1 | 1:147:A:ASP:HB2 | 20 | 0.86 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 1 | 0.86 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 5 | 0.86 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 5 | 0.86 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 1 | 0.86 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 6 | 0.86 |
| (4,166) | 1:171:A:VAL:H | 1:168:A:ILE:HG13 | 14 | 0.86 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 10 | 0.86 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 15 | 0.86 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD13 | 10 | 0.86 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 2 | 0.86 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 4 | 0.86 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 16 | 0.86 |
| (2,3421) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 4 | 0.86 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 10 | 0.86 |
| (2,3421) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 14 | 0.86 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 15 | 0.86 |
| (2,1868) | 1:97:A:LEU:HD21 | 1:95:A:ALA:HB1 | 1 | 0.86 |
| (2,1865) | 1:109:A:ILE:HD11 | 1:144:A:LEU:HD13 | 3 | 0.86 |
| (2,1851) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD13 | 6 | 0.86 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 3 | 0.86 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 12 | 0.86 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 17 | 0.86 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 11 | 0.86 |
| (2,1500) | 1:11:A:LEU:HD12 | 1:38:A:LEU:HA | 14 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 15 | 0.86 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 2 | 0.86 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 3 | 0.86 |
| (2,1492) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 9 | 0.86 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 7 | 0.86 |
| (2,1473) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 13 | 0.86 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 1 | 0.86 |
| (2,1291) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 12 | 0.86 |
| (2,1217) | 1:177:A:LYS:HE2 | 1:177:A:LYS:HB2 | 12 | 0.86 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 11 | 0.86 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 18 | 0.86 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD13 | 5 | 0.85 |
| (4,332) | 1:37:A:LEU:HD13 | 1:41:A:MET:HB2 | 18 | 0.85 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 2 | 0.85 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 18 | 0.85 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 5 | 0.85 |
| (4,6) | 1:65:A:PHE:HE1 | 1:74:A:ILE:HG23 | 1 | 0.85 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD21 | 6 | 0.85 |
| (2,3771) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HB2 | 2 | 0.85 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 9 | 0.85 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 10 | 0.85 |
| (2,3771) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HB2 | 15 | 0.85 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 12 | 0.85 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 7 | 0.85 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 11 | 0.85 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 2 | 0.85 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 3 | 0.85 |
| (2,3421) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 17 | 0.85 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 2 | 0.85 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 10 | 0.85 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE1 | 14 | 0.85 |
| (2,1807) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 2 | 0.85 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 4 | 0.85 |
| (2,1549) | 1:37:A:LEU:HD12 | 1:41:A:MET:HG2 | 19 | 0.85 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 1 | 0.85 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 4 | 0.85 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 4 | 0.85 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 15 | 0.85 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 11 | 0.85 |
| (2,816) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 15 | 0.85 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 5 | 0.85 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD22 | 6 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,450) | 1:97:A:LEU:HD21 | 1:124:A:LEU:HD22 | 10 | 0.84 |
| (4,378) | 1:24:A:LEU:HA | 1:15:A:LEU:HB2 | 3 | 0.84 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 12 | 0.84 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 9 | 0.84 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 16 | 0.84 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 2 | 0.84 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 16 | 0.84 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 4 | 0.84 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 10 | 0.84 |
| (2,3813) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 17 | 0.84 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 11 | 0.84 |
| (2,3527) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 6 | 0.84 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 17 | 0.84 |
| (2,3421) | 1:38:A:LEU:HD11 | 1:38:A:LEU:H | 7 | 0.84 |
| (2,3421) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 11 | 0.84 |
| (2,3421) | 1:38:A:LEU:HD11 | 1:38:A:LEU:H | 18 | 0.84 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 14 | 0.84 |
| (2,1899) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 1 | 0.84 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 2 | 0.84 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 14 | 0.84 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 18 | 0.84 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 20 | 0.84 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 16 | 0.84 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 11 | 0.84 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 15 | 0.84 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 16 | 0.84 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 17 | 0.84 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 14 | 0.84 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 17 | 0.84 |
| (2,1291) | 1:84:A:VAL:HG13 | 1:84:A:VAL:H | 3 | 0.84 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 12 | 0.84 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 2 | 0.84 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 14 | 0.84 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 6 | 0.84 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 20 | 0.83 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 5 | 0.83 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 17 | 0.83 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 11 | 0.83 |
| (4,222) | 1:57:A:VAL:HG22 | 1:74:A:ILE:HB | 17 | 0.83 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 20 | 0.83 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 9 | 0.83 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 16 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 14 | 0.83 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 17 | 0.83 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD21 | 9 | 0.83 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 17 | 0.83 |
| (2,3964) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H6N | 13 | 0.83 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 15 | 0.83 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 15 | 0.83 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 17 | 0.83 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 5 | 0.83 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 8 | 0.83 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 13 | 0.83 |
| (2,1869) | 1:97:A:LEU:HD23 | 1:96:A:VAL:HB | 2 | 0.83 |
| (2,1865) | 1:109:A:ILE:HD11 | 1:144:A:LEU:HD13 | 16 | 0.83 |
| (2,1856) | 1:22:A:ILE:HD12 | 1:14:A:VAL:HG23 | 5 | 0.83 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 19 | 0.83 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 20 | 0.83 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 2 | 0.83 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 6 | 0.83 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 9 | 0.83 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 2 | 0.83 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG11 | 17 | 0.83 |
| (2,1610) | 1:13:A:LEU:HG | 1:17:A:HIS:HB2 | 5 | 0.83 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 6 | 0.83 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 2 | 0.83 |
| (2,1549) | 1:37:A:LEU:HD13 | 1:41:A:MET:HG2 | 17 | 0.83 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 17 | 0.83 |
| (2,1490) | 1:167:A:LEU:HD13 | 1:166:A:TRP:HA | 4 | 0.83 |
| (2,1473) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 11 | 0.83 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 2 | 0.83 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 6 | 0.83 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 15 | 0.83 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 3 | 0.83 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 11 | 0.83 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 16 | 0.83 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 13 | 0.83 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 17 | 0.83 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 6 | 0.83 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 17 | 0.83 |
| (4,458) | 1:50:A:MET:HE2 | 1:51:A:GLU:HA | 14 | 0.82 |
| (4,450) | 1:97:A:LEU:HD21 | 1:124:A:LEU:HD23 | 4 | 0.82 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 6 | 0.82 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 11 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB2 | 9 | 0.82 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 20 | 0.82 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 10 | 0.82 |
| (4,204) | 1:173:A:ALA:HB1 | 1:111:A:LYS:HG2 | 6 | 0.82 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 19 | 0.82 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 9 | 0.82 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 14 | 0.82 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 12 | 0.82 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD11 | 11 | 0.82 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 4 | 0.82 |
| (4,6) | 1:65:A:PHE:HE1 | 1:74:A:ILE:HG23 | 3 | 0.82 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 19 | 0.82 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 16 | 0.82 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 8 | 0.82 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 8 | 0.82 |
| (2,3462) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 7 | 0.82 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 20 | 0.82 |
| (2,3421) | 1:38:A:LEU:HD13 | 1:38:A:LEU:H | 12 | 0.82 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 19 | 0.82 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 16 | 0.82 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 8 | 0.82 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 14 | 0.82 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 7 | 0.82 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 11 | 0.82 |
| (2,1845) | 1:176:A:ILE:HB | 1:110:A:LEU:HD11 | 14 | 0.82 |
| (2,1845) | 1:110:A:LEU:HD13 | 1:176:A:ILE:HB | 15 | 0.82 |
| (2,1794) | 1:117:A:MET:HE3 | 1:117:A:MET:HB2 | 12 | 0.82 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 5 | 0.82 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 11 | 0.82 |
| (2,1549) | 1:37:A:LEU:HD12 | 1:41:A:MET:HG2 | 13 | 0.82 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 16 | 0.82 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 17 | 0.82 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 10 | 0.82 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 12 | 0.82 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 18 | 0.82 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 19 | 0.82 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 7 | 0.82 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 5 | 0.82 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 8 | 0.82 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 12 | 0.82 |
| (2,954) | 1:56:A:ILE:HG21 | 1:57:A:VAL:H | 14 | 0.82 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 20 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 1 | 0.82 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 6 | 0.82 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 8 | 0.82 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 14 | 0.82 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 9 | 0.82 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 1 | 0.82 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD22 | 8 | 0.81 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD22 | 17 | 0.81 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 2 | 0.81 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 17 | 0.81 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 19 | 0.81 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 3 | 0.81 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 14 | 0.81 |
| (4,320) | 1:151:A:MET:HE1 | 1:147:A:ASP:HB2 | 14 | 0.81 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 6 | 0.81 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 11 | 0.81 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 17 | 0.81 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 6 | 0.81 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 5 | 0.81 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 2 | 0.81 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 11 | 0.81 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 15 | 0.81 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 20 | 0.81 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 16 | 0.81 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 20 | 0.81 |
| (2,3847) | 1:41:A:MET:HE3 | 1:46:A:HIS:HA | 17 | 0.81 |
| (2,3784) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 12 | 0.81 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 14 | 0.81 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 4 | 0.81 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 2 | 0.81 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 19 | 0.81 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 2 | 0.81 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 15 | 0.81 |
| (2,3462) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 14 | 0.81 |
| (2,2348) | 1:156:A:PHE:H | 1:168:A:ILE:HD11 | 5 | 0.81 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 5 | 0.81 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 14 | 0.81 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 4 | 0.81 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 4 | 0.81 |
| (2,1807) | 1:151:A:MET:HE3 | 1:174:A:GLU:HG2 | 7 | 0.81 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 4 | 0.81 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 8 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 10 | 0.81 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 15 | 0.81 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 17 | 0.81 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG12 | 19 | 0.81 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 10 | 0.81 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 15 | 0.81 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 3 | 0.81 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 5 | 0.81 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 9 | 0.81 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 11 | 0.81 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 15 | 0.81 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 20 | 0.81 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 7 | 0.81 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 7 | 0.81 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 7 | 0.81 |
| (2,954) | 1:56:A:ILE:HG23 | 1:57:A:VAL:H | 9 | 0.81 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 16 | 0.81 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 17 | 0.81 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 14 | 0.81 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 16 | 0.8 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 9 | 0.8 |
| (4,313) | 1:96:A:VAL:HG13 | 1:145:A:SER:HA | 6 | 0.8 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 15 | 0.8 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD11 | 15 | 0.8 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD23 | 4 | 0.8 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 1 | 0.8 |
| (2,3847) | 1:41:A:MET:HE3 | 1:46:A:HIS:HA | 16 | 0.8 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 13 | 0.8 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 17 | 0.8 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 19 | 0.8 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 17 | 0.8 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 11 | 0.8 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 7 | 0.8 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 7 | 0.8 |
| (2,2221) | 1:168:A:ILE:HD12 | 1:157:A:ASP:H | 17 | 0.8 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 17 | 0.8 |
| (2,1865) | 1:109:A:ILE:HD11 | 1:144:A:LEU:HD13 | 10 | 0.8 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 10 | 0.8 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 1 | 0.8 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 13 | 0.8 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 16 | 0.8 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 11 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 18 | 0.8 |
| (2,1554) | 1:38:A:LEU:HD21 | 1:50:A:MET:HG2 | 14 | 0.8 |
| (2,1473) | 1:110:A:LEU:HD13 | 1:110:A:LEU:H | 9 | 0.8 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 14 | 0.8 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 7 | 0.8 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 8 | 0.8 |
| (2,1434) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 13 | 0.8 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 13 | 0.8 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 17 | 0.8 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 19 | 0.8 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 4 | 0.8 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 6 | 0.8 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 7 | 0.8 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD23 | 7 | 0.79 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD21 | 15 | 0.79 |
| (4,332) | 1:37:A:LEU:HD13 | 1:41:A:MET:HB2 | 6 | 0.79 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 18 | 0.79 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 15 | 0.79 |
| (4,204) | 1:173:A:ALA:HB1 | 1:111:A:LYS:HG3 | 16 | 0.79 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 19 | 0.79 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 20 | 0.79 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 16 | 0.79 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 2 | 0.79 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 16 | 0.79 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 4 | 0.79 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 6 | 0.79 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 19 | 0.79 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 20 | 0.79 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 9 | 0.79 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 17 | 0.79 |
| (2,3500) | 1:144:A:LEU:HD22 | 1:145:A:SER:HB2 | 9 | 0.79 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 3 | 0.79 |
| (2,3421) | 1:38:A:LEU:HD12 | 1:38:A:LEU:H | 16 | 0.79 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 4 | 0.79 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 7 | 0.79 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 8 | 0.79 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 9 | 0.79 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 11 | 0.79 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 12 | 0.79 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 13 | 0.79 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 19 | 0.79 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 3 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 9 | 0.79 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 16 | 0.79 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG23 | 8 | 0.79 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 10 | 0.79 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 16 | 0.79 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 3 | 0.79 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 9 | 0.79 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 1 | 0.79 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 3 | 0.79 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG12 | 14 | 0.79 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 9 | 0.79 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 6 | 0.79 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 17 | 0.79 |
| (2,1236) | 1:151:A:MET:HE3 | 1:156:A:PHE:HZ | 5 | 0.79 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 12 | 0.79 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 6 | 0.79 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 11 | 0.79 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 9 | 0.79 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 15 | 0.79 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 17 | 0.79 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 8 | 0.79 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD23 | 3 | 0.78 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD22 | 15 | 0.78 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 16 | 0.78 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 12 | 0.78 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 16 | 0.78 |
| (4,204) | 1:173:A:ALA:HB3 | 1:111:A:LYS:HG3 | 14 | 0.78 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 3 | 0.78 |
| (4,184) | 1:105:A:ASN:H | 1:136:A:MET:H | 19 | 0.78 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 6 | 0.78 |
| (4,160) | 1:22:A:ILE:HD13 | 1:22:A:ILE:H | 20 | 0.78 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 16 | 0.78 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 8 | 0.78 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 3 | 0.78 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 16 | 0.78 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 4 | 0.78 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 2 | 0.78 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 3 | 0.78 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD23 | 13 | 0.78 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 6 | 0.78 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 2 | 0.78 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 6 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 10 | 0.78 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 14 | 0.78 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 16 | 0.78 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 17 | 0.78 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 18 | 0.78 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 11 | 0.78 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 14 | 0.78 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 9 | 0.78 |
| (2,1847) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 20 | 0.78 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 2 | 0.78 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 6 | 0.78 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 2 | 0.78 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 6 | 0.78 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 7 | 0.78 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 11 | 0.78 |
| (2,1495) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 18 | 0.78 |
| (2,1492) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 1 | 0.78 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 12 | 0.78 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 13 | 0.78 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 4 | 0.78 |
| (2,1157) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HD1 | 13 | 0.78 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 1 | 0.78 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 2 | 0.78 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 3 | 0.78 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 15 | 0.78 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 19 | 0.78 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 3 | 0.78 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 16 | 0.78 |
| (2,300) | 1:153:A:ASP:H | 1:95:A:ALA:HB1 | 5 | 0.78 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 8 | 0.78 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 15 | 0.78 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 8 | 0.78 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 15 | 0.78 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD22 | 1 | 0.77 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 12 | 0.77 |
| (4,378) | 1:24:A:LEU:HA | 1:15:A:LEU:HB2 | 1 | 0.77 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 3 | 0.77 |
| (4,311) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 13 | 0.77 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 17 | 0.77 |
| (4,283) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 3 | 0.77 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 20 | 0.77 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 4 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 11 | 0.77 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 15 | 0.77 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 9 | 0.77 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 11 | 0.77 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 14 | 0.77 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 4 | 0.77 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 5 | 0.77 |
| (2,3813) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD11 | 12 | 0.77 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 5 | 0.77 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 14 | 0.77 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 20 | 0.77 |
| (2,3416) | 1:143:A:VAL:HG13 | 1:143:A:VAL:H | 15 | 0.77 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 18 | 0.77 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 15 | 0.77 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 8 | 0.77 |
| (2,1875) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 11 | 0.77 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 7 | 0.77 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 15 | 0.77 |
| (2,1740) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 5 | 0.77 |
| (2,1554) | 1:38:A:LEU:HD21 | 1:50:A:MET:HG2 | 20 | 0.77 |
| (2,1549) | 1:37:A:LEU:HD12 | 1:41:A:MET:HG2 | 20 | 0.77 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 20 | 0.77 |
| (2,1473) | 1:110:A:LEU:HD13 | 1:110:A:LEU:H | 5 | 0.77 |
| (2,1473) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 10 | 0.77 |
| (2,1388) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 5 | 0.77 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 20 | 0.77 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 8 | 0.77 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 20 | 0.77 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 7 | 0.77 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 3 | 0.77 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 13 | 0.77 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 19 | 0.77 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 11 | 0.77 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 5 | 0.77 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD21 | 9 | 0.76 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD23 | 13 | 0.76 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD22 | 20 | 0.76 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 16 | 0.76 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD21 | 1 | 0.76 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 14 | 0.76 |
| (4,332) | 1:37:A:LEU:HD12 | 1:41:A:MET:HB2 | 7 | 0.76 |
| (4,204) | 1:173:A:ALA:HB1 | 1:111:A:LYS:HG3 | 17 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 2 | 0.76 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 3 | 0.76 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 7 | 0.76 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 8 | 0.76 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 17 | 0.76 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 17 | 0.76 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 19 | 0.76 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 7 | 0.76 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 13 | 0.76 |
| (4,6) | 1:65:A:PHE:HE1 | 1:74:A:ILE:HG23 | 20 | 0.76 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 3 | 0.76 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 16 | 0.76 |
| (2,3784) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 17 | 0.76 |
| (2,3772) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 20 | 0.76 |
| (2,3657) | 1:63:A:LYS:HG2 | 1:62:A:LYS:HA | 6 | 0.76 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 17 | 0.76 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 8 | 0.76 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 13 | 0.76 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 16 | 0.76 |
| (2,3524) | 1:13:A:LEU:HD11 | 1:18:A:ASN:HB2 | 12 | 0.76 |
| (2,3466) | 1:97:A:LEU:HD22 | 1:166:A:TRP:HB2 | 9 | 0.76 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 10 | 0.76 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 7 | 0.76 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 14 | 0.76 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 6 | 0.76 |
| (2,1875) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 10 | 0.76 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 1 | 0.76 |
| (2,1845) | 1:176:A:ILE:HB | 1:110:A:LEU:HD11 | 5 | 0.76 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 11 | 0.76 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 10 | 0.76 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 13 | 0.76 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 12 | 0.76 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 19 | 0.76 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 4 | 0.76 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 6 | 0.76 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 10 | 0.76 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 11 | 0.76 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 13 | 0.76 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 1 | 0.76 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 3 | 0.76 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 5 | 0.76 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 10 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 15 | 0.76 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 16 | 0.76 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 15 | 0.76 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 2 | 0.76 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 18 | 0.76 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 7 | 0.76 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 16 | 0.76 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 9 | 0.76 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 6 | 0.76 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 9 | 0.76 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 16 | 0.76 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 17 | 0.76 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 20 | 0.76 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD23 | 19 | 0.75 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 12 | 0.75 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 4 | 0.75 |
| (4,332) | 1:37:A:LEU:HD13 | 1:41:A:MET:HB2 | 8 | 0.75 |
| (4,320) | 1:151:A:MET:HE1 | 1:147:A:ASP:HB2 | 13 | 0.75 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 13 | 0.75 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 12 | 0.75 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 18 | 0.75 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD13 | 12 | 0.75 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 14 | 0.75 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD11 | 16 | 0.75 |
| (4,160) | 1:22:A:ILE:HD11 | 1:22:A:ILE:H | 3 | 0.75 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 8 | 0.75 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 18 | 0.75 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 6 | 0.75 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 17 | 0.75 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 20 | 0.75 |
| (2,3790) | 1:34:A:VAL:HG12 | 1:50:A:MET:HE1 | 18 | 0.75 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 13 | 0.75 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 15 | 0.75 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 10 | 0.75 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 8 | 0.75 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 9 | 0.75 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 20 | 0.75 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 17 | 0.75 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 12 | 0.75 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 10 | 0.75 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 12 | 0.75 |
| (2,1884) | 1:41:A:MET:HE1 | 1:46:A:HIS:HA | 7 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1875) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 5 | 0.75 |
| (2,1871) | 1:97:A:LEU:HD22 | 1:151:A:MET:HG3 | 2 | 0.75 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 9 | 0.75 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 15 | 0.75 |
| (2,1823) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 12 | 0.75 |
| (2,1790) | 1:144:A:LEU:HG | 1:178:A:VAL:HG12 | 7 | 0.75 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 6 | 0.75 |
| (2,1742) | 1:110:A:LEU:HD11 | 1:173:A:ALA:HA | 14 | 0.75 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 5 | 0.75 |
| (2,1522) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 1 | 0.75 |
| (2,1495) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 4 | 0.75 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 13 | 0.75 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 15 | 0.75 |
| (2,1361) | 1:177:A:LYS:HE2 | 1:147:A:ASP:H | 2 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 2 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 6 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 7 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 8 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 11 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 13 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 17 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 18 | 0.75 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 19 | 0.75 |
| (2,288) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 9 | 0.75 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 19 | 0.75 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 7 | 0.75 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 4 | 0.75 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 7 | 0.75 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 10 | 0.75 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 12 | 0.75 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 13 | 0.75 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 14 | 0.75 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 19 | 0.75 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD23 | 18 | 0.74 |
| (4,431) | 1:13:A:LEU:HG | 1:13:A:LEU:HD12 | 10 | 0.74 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 15 | 0.74 |
| (4,402) | 1:42:A:LYS:HG3 | 1:42:A:LYS:HE3 | 14 | 0.74 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 1 | 0.74 |
| (4,259) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 4 | 0.74 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 19 | 0.74 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 10 | 0.74 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 9 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 4 | 0.74 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 4 | 0.74 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 4 | 0.74 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 20 | 0.74 |
| (2,3813) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD11 | 4 | 0.74 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 18 | 0.74 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 4 | 0.74 |
| (2,3790) | 1:34:A:VAL:HG12 | 1:50:A:MET:HE2 | 1 | 0.74 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 15 | 0.74 |
| (2,3527) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 1 | 0.74 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 16 | 0.74 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 16 | 0.74 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 6 | 0.74 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 8 | 0.74 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 17 | 0.74 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 4 | 0.74 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 5 | 0.74 |
| (2,1884) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 8 | 0.74 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 2 | 0.74 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 16 | 0.74 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 3 | 0.74 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 4 | 0.74 |
| (2,1742) | 1:110:A:LEU:HD13 | 1:173:A:ALA:HA | 15 | 0.74 |
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 18 | 0.74 |
| (2,1610) | 1:13:A:LEU:HG | 1:17:A:HIS:HB2 | 12 | 0.74 |
| (2,1601) | 1:41:A:MET:HE2 | 1:10:A:PHE:HB3 | 15 | 0.74 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 5 | 0.74 |
| (2,1549) | 1:37:A:LEU:HD11 | 1:41:A:MET:HG2 | 10 | 0.74 |
| (2,1549) | 1:37:A:LEU:HD11 | 1:41:A:MET:HG2 | 14 | 0.74 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 16 | 0.74 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 12 | 0.74 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 2 | 0.74 |
| (2,1426) | 1:86:A:LEU:HD12 | 1:88:A:TYR:HD1 | 20 | 0.74 |
| (2,1425) | 1:56:A:ILE:HG23 | 1:65:A:PHE:HD1 | 9 | 0.74 |
| (2,1424) | 1:56:A:ILE:HG23 | 1:65:A:PHE:HE1 | 9 | 0.74 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 11 | 0.74 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 2 | 0.74 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 5 | 0.74 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 7 | 0.74 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 8 | 0.74 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 13 | 0.74 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 17 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 3 | 0.74 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 2 | 0.74 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 5 | 0.74 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 18 | 0.74 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 4 | 0.73 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD22 | 6 | 0.73 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 11 | 0.73 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD23 | 12 | 0.73 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD22 | 13 | 0.73 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 14 | 0.73 |
| (4,431) | 1:13:A:LEU:HG | 1:13:A:LEU:HD12 | 18 | 0.73 |
| (4,431) | 1:13:A:LEU:HG | 1:13:A:LEU:HD12 | 19 | 0.73 |
| (4,414) | 1:44:A:LYS:HB3 | 1:14:A:VAL:HG13 | 17 | 0.73 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 4 | 0.73 |
| (4,338) | 1:111:A:LYS:HD3 | 1:104:A:LYS:HA | 1 | 0.73 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 3 | 0.73 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 7 | 0.73 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 14 | 0.73 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 18 | 0.73 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 4 | 0.73 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 6 | 0.73 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 8 | 0.73 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD12 | 10 | 0.73 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 9 | 0.73 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 19 | 0.73 |
| (4,160) | 1:22:A:ILE:HD12 | 1:22:A:ILE:H | 1 | 0.73 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 7 | 0.73 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 14 | 0.73 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 6 | 0.73 |
| (2,3657) | 1:63:A:LYS:HG2 | 1:62:A:LYS:HA | 17 | 0.73 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 7 | 0.73 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 11 | 0.73 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 6 | 0.73 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 10 | 0.73 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 14 | 0.73 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 18 | 0.73 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 16 | 0.73 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 1 | 0.73 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 15 | 0.73 |
| (2,3416) | 1:143:A:VAL:HG11 | 1:143:A:VAL:H | 8 | 0.73 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 19 | 0.73 |
| (2,3416) | 1:143:A:VAL:HG11 | 1:143:A:VAL:H | 20 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 14 | 0.73 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 17 | 0.73 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 7 | 0.73 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 13 | 0.73 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 10 | 0.73 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 1 | 0.73 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB3 | 7 | 0.73 |
| (2,1783) | 1:44:A:LYS:HG3 | 1:21:A:LEU:HD22 | 20 | 0.73 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG11 | 4 | 0.73 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 19 | 0.73 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 4 | 0.73 |
| (2,1511) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 9 | 0.73 |
| (2,1490) | 1:167:A:LEU:HD12 | 1:166:A:TRP:HA | 11 | 0.73 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 7 | 0.73 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 18 | 0.73 |
| (2,1375) | 1:41:A:MET:HE2 | 1:10:A:PHE:HD1 | 5 | 0.73 |
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 3 | 0.73 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 9 | 0.73 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 14 | 0.73 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 3 | 0.73 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 9 | 0.73 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 4 | 0.73 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 9 | 0.73 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 13 | 0.73 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 16 | 0.73 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 17 | 0.73 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 16 | 0.73 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 2 | 0.73 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 1 | 0.73 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 5 | 0.72 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 7 | 0.72 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 8 | 0.72 |
| (4,402) | 1:6:A:LYS:HE2 | 1:6:A:LYS:HG3 | 9 | 0.72 |
| (4,311) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 6 | 0.72 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 19 | 0.72 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 14 | 0.72 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 7 | 0.72 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 7 | 0.72 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 9 | 0.72 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD23 | 15 | 0.72 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 8 | 0.72 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 17 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 19 | 0.72 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 4 | 0.72 |
| (2,3481) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 9 | 0.72 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 10 | 0.72 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 3 | 0.72 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 2 | 0.72 |
| (2,3265) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 11 | 0.72 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 11 | 0.72 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 7 | 0.72 |
| (2,1884) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 6 | 0.72 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 16 | 0.72 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 12 | 0.72 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 2 | 0.72 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 9 | 0.72 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 9 | 0.72 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 18 | 0.72 |
| (2,1599) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 2 | 0.72 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 7 | 0.72 |
| (2,1512) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 8 | 0.72 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 1 | 0.72 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 2 | 0.72 |
| (2,1482) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 6 | 0.72 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 8 | 0.72 |
| (2,1190) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HA | 14 | 0.72 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 2 | 0.72 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 7 | 0.72 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 12 | 0.72 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 1 | 0.72 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 5 | 0.72 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 11 | 0.72 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 4 | 0.72 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 12 | 0.72 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 17 | 0.72 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 9 | 0.72 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD22 | 9 | 0.71 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 17 | 0.71 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD22 | 20 | 0.71 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 3 | 0.71 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 13 | 0.71 |
| (4,320) | 1:151:A:MET:HE3 | 1:158:A:PHE:HB3 | 6 | 0.71 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 13 | 0.71 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 3 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 2 | 0.71 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 9 | 0.71 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD11 | 5 | 0.71 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 3 | 0.71 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 7 | 0.71 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 20 | 0.71 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 12 | 0.71 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 20 | 0.71 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 20 | 0.71 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 6 | 0.71 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 18 | 0.71 |
| (2,3657) | 1:63:A:LYS:HG2 | 1:62:A:LYS:HA | 13 | 0.71 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 16 | 0.71 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 10 | 0.71 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 19 | 0.71 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 12 | 0.71 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 3 | 0.71 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 9 | 0.71 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 15 | 0.71 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 14 | 0.71 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 1 | 0.71 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 11 | 0.71 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 16 | 0.71 |
| (2,1845) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 18 | 0.71 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 14 | 0.71 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 20 | 0.71 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 5 | 0.71 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 16 | 0.71 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 4 | 0.71 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 5 | 0.71 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 9 | 0.71 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 3 | 0.71 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 6 | 0.71 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 8 | 0.71 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 17 | 0.71 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 12 | 0.71 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 4 | 0.71 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 7 | 0.71 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 17 | 0.71 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 19 | 0.71 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 8 | 0.71 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 20 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 13 | 0.71 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 15 | 0.71 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 20 | 0.71 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 11 | 0.71 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 18 | 0.71 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 11 | 0.71 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 13 | 0.71 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 11 | 0.71 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 7 | 0.71 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 3 | 0.71 |
| (2,35) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 11 | 0.71 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 8 | 0.7 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD23 | 2 | 0.7 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD23 | 3 | 0.7 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 16 | 0.7 |
| (4,409) | 1:4:A:MET:HE1 | 1:59:A:THR:HG23 | 5 | 0.7 |
| (4,368) | 1:20:A:ALA:HB3 | 1:22:A:ILE:HB | 1 | 0.7 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 4 | 0.7 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 7 | 0.7 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 10 | 0.7 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 20 | 0.7 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 6 | 0.7 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 7 | 0.7 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 9 | 0.7 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 7 | 0.7 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 10 | 0.7 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 1 | 0.7 |
| (2,3784) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE1 | 20 | 0.7 |
| (2,3772) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 2 | 0.7 |
| (2,3761) | 1:117:A:MET:HE3 | 1:117:A:MET:HB2 | 12 | 0.7 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 8 | 0.7 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 14 | 0.7 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 9 | 0.7 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 16 | 0.7 |
| (2,3570) | 1:4:A:MET:HE2 | 1:52:A:GLU:HA | 19 | 0.7 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 6 | 0.7 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 11 | 0.7 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 9 | 0.7 |
| (2,3462) | 1:168:A:ILE:HD13 | 1:175:A:PHE:HB3 | 18 | 0.7 |
| (2,3416) | 1:143:A:VAL:HG13 | 1:143:A:VAL:H | 1 | 0.7 |
| (2,3416) | 1:143:A:VAL:HG11 | 1:143:A:VAL:H | 4 | 0.7 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 17 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 1 | 0.7 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 4 | 0.7 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 10 | 0.7 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 6 | 0.7 |
| (2,3265) | 1:84:A:VAL:HG13 | 1:84:A:VAL:H | 18 | 0.7 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 2 | 0.7 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 5 | 0.7 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 8 | 0.7 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 10 | 0.7 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 12 | 0.7 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 18 | 0.7 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 20 | 0.7 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 17 | 0.7 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 20 | 0.7 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 7 | 0.7 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 16 | 0.7 |
| (2,1856) | 1:22:A:ILE:HD12 | 1:14:A:VAL:HG22 | 7 | 0.7 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 3 | 0.7 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 4 | 0.7 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 16 | 0.7 |
| (2,1823) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 17 | 0.7 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 1 | 0.7 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 6 | 0.7 |
| (2,1807) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 16 | 0.7 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 8 | 0.7 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 12 | 0.7 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 13 | 0.7 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 3 | 0.7 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 15 | 0.7 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 15 | 0.7 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 18 | 0.7 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 20 | 0.7 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 18 | 0.7 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 15 | 0.7 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 16 | 0.7 |
| (2,1377) | 1:4:A:MET:HE2 | 1:55:A:HIS:HD2 | 20 | 0.7 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 1 | 0.7 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 11 | 0.7 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 6 | 0.7 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 10 | 0.7 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 12 | 0.7 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 1 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 10 | 0.7 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 6 | 0.7 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 16 | 0.7 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 7 | 0.7 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 10 | 0.7 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 19 | 0.7 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 4 | 0.7 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 17 | 0.7 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 2 | 0.7 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 15 | 0.7 |
| (4,437) | 1:178:A:VAL:HG23 | 1:177:A:LYS:HG2 | 19 | 0.69 |
| (4,431) | 1:37:A:LEU:HG | 1:37:A:LEU:HD21 | 1 | 0.69 |
| (4,332) | 1:37:A:LEU:HD12 | 1:41:A:MET:HB2 | 19 | 0.69 |
| (4,320) | 1:151:A:MET:HE1 | 1:147:A:ASP:HB2 | 8 | 0.69 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 9 | 0.69 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 8 | 0.69 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 1 | 0.69 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 13 | 0.69 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 16 | 0.69 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 18 | 0.69 |
| (4,95) | 1:51:A:GLU:H | 1:58:A:GLU:HG3 | 14 | 0.69 |
| (2,3657) | 1:63:A:LYS:HG3 | 1:62:A:LYS:HA | 19 | 0.69 |
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 5 | 0.69 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 2 | 0.69 |
| (2,3524) | 1:13:A:LEU:HD11 | 1:18:A:ASN:HB2 | 5 | 0.69 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 13 | 0.69 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 10 | 0.69 |
| (2,3346) | 1:4:A:MET:HE2 | 1:55:A:HIS:HD2 | 20 | 0.69 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 1 | 0.69 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 13 | 0.69 |
| (2,3265) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 14 | 0.69 |
| (2,3211) | 1:151:A:MET:HE2 | 1:156:A:PHE:HZ | 9 | 0.69 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 5 | 0.69 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 6 | 0.69 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 14 | 0.69 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 19 | 0.69 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 2 | 0.69 |
| (2,1935) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 13 | 0.69 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 13 | 0.69 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 3 | 0.69 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 2 | 0.69 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 17 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1690) | 1:63:A:LYS:HG2 | 1:62:A:LYS:HA | 6 | 0.69 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 12 | 0.69 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 6 | 0.69 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 19 | 0.69 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 4 | 0.69 |
| (2,1291) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 7 | 0.69 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 9 | 0.69 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 18 | 0.69 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 4 | 0.69 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 14 | 0.69 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 9 | 0.69 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 14 | 0.69 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 14 | 0.69 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 14 | 0.69 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 4 | 0.69 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 12 | 0.69 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 1 | 0.69 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 10 | 0.69 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 16 | 0.69 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 3 | 0.69 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 3 | 0.68 |
| (4,437) | 1:178:A:VAL:HG23 | 1:177:A:LYS:HG2 | 2 | 0.68 |
| (4,437) | 1:178:A:VAL:HG23 | 1:177:A:LYS:HG2 | 5 | 0.68 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 11 | 0.68 |
| (4,428) | 1:108:A:LEU:HD12 | 1:107:A:ASP:HB2 | 4 | 0.68 |
| (4,407) | 1:178:A:VAL:HB | 1:110:A:LEU:HD22 | 4 | 0.68 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 7 | 0.68 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 9 | 0.68 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 8 | 0.68 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 8 | 0.68 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 14 | 0.68 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 13 | 0.68 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 10 | 0.68 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 15 | 0.68 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 18 | 0.68 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 12 | 0.68 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD21 | 20 | 0.68 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 2 | 0.68 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 12 | 0.68 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 18 | 0.68 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 18 | 0.68 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 9 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 14 | 0.68 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 17 | 0.68 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 9 | 0.68 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 19 | 0.68 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 4 | 0.68 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 9 | 0.68 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 18 | 0.68 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 20 | 0.68 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 16 | 0.68 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 6 | 0.68 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 17 | 0.68 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 19 | 0.68 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 20 | 0.68 |
| (2,1495) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 13 | 0.68 |
| (2,1492) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 3 | 0.68 |
| (2,1492) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 19 | 0.68 |
| (2,1473) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 14 | 0.68 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 1 | 0.68 |
| (2,1378) | 1:50:A:MET:HE1 | 1:67:A:PHE:HZ | 14 | 0.68 |
| (2,1297) | 1:57:A:VAL:HG13 | 1:67:A:PHE:HB3 | 5 | 0.68 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 12 | 0.68 |
| (2,1297) | 1:57:A:VAL:HG13 | 1:67:A:PHE:HB3 | 13 | 0.68 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 2 | 0.68 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 3 | 0.68 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 19 | 0.68 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 16 | 0.68 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 16 | 0.68 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 11 | 0.68 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 13 | 0.68 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 4 | 0.68 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 6 | 0.68 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 8 | 0.68 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 9 | 0.68 |
| (2,342) | 1:41:A:MET:H | 1:41:A:MET:HG2 | 16 | 0.68 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 1 | 0.68 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 3 | 0.68 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 6 | 0.68 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 18 | 0.68 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 15 | 0.68 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 18 | 0.68 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 16 | 0.67 |
| (4,338) | 1:111:A:LYS:HD3 | 1:104:A:LYS:HA | 20 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,332) | 1:37:A:LEU:HD11 | 1:41:A:MET:HB2 | 4 | 0.67 |
| (4,332) | 1:37:A:LEU:HD12 | 1:41:A:MET:HB2 | 13 | 0.67 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 1 | 0.67 |
| (4,259) | 1:117:A:MET:HE3 | 2:201:A:NAD:H2A | 9 | 0.67 |
| (4,227) | 1:8:A:SER:HB3 | 1:55:A:HIS:HD2 | 15 | 0.67 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 9 | 0.67 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 16 | 0.67 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 15 | 0.67 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 1 | 0.67 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 5 | 0.67 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 8 | 0.67 |
| (4,190) | 1:60:A:ASN:H | 1:73:A:LYS:H | 17 | 0.67 |
| (4,166) | 1:171:A:VAL:H | 1:168:A:ILE:HG13 | 2 | 0.67 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 6 | 0.67 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 13 | 0.67 |
| (2,3964) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H6N | 2 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 3 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD11 | 11 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 13 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 15 | 0.67 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 16 | 0.67 |
| (2,3784) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 2 | 0.67 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 19 | 0.67 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 14 | 0.67 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 1 | 0.67 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 12 | 0.67 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 6 | 0.67 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 8 | 0.67 |
| (2,3462) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 4 | 0.67 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 19 | 0.67 |
| (2,3459) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 11 | 0.67 |
| (2,3416) | 1:143:A:VAL:HG13 | 1:143:A:VAL:H | 16 | 0.67 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 2 | 0.67 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 6 | 0.67 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 18 | 0.67 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 19 | 0.67 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 4 | 0.67 |
| (2,3271) | 1:57:A:VAL:HG13 | 1:67:A:PHE:HB3 | 5 | 0.67 |
| (2,3271) | 1:57:A:VAL:HG13 | 1:67:A:PHE:HB3 | 13 | 0.67 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 7 | 0.67 |
| (2,2784) | 1:53:A:LEU:HD22 | 1:53:A:LEU:H | 6 | 0.67 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 10 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 19 | 0.67 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 4 | 0.67 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 17 | 0.67 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD12 | 20 | 0.67 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 19 | 0.67 |
| (2,1865) | 1:109:A:ILE:HD11 | 1:144:A:LEU:HD13 | 15 | 0.67 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 13 | 0.67 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 2 | 0.67 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 9 | 0.67 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 13 | 0.67 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 15 | 0.67 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 1 | 0.67 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 7 | 0.67 |
| (2,1742) | 1:110:A:LEU:HD11 | 1:173:A:ALA:HA | 9 | 0.67 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 2 | 0.67 |
| (2,1535) | 1:22:A:ILE:HG21 | 1:44:A:LYS:HE3 | 16 | 0.67 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 17 | 0.67 |
| (2,1412) | 1:66:A:ALA:HB2 | 1:31:A:TRP:HZ3 | 12 | 0.67 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 19 | 0.67 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 3 | 0.67 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 18 | 0.67 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 11 | 0.67 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 17 | 0.67 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 18 | 0.67 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 4 | 0.67 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB3 | 5 | 0.67 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 9 | 0.67 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 5 | 0.67 |
| (2,255) | 1:168:A:ILE:HD12 | 1:157:A:ASP:H | 17 | 0.67 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 8 | 0.67 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 12 | 0.67 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 19 | 0.67 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 20 | 0.67 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 17 | 0.67 |
| (4,450) | 1:97:A:LEU:HD23 | 1:124:A:LEU:HD23 | 17 | 0.66 |
| (4,409) | 1:4:A:MET:HE3 | 1:59:A:THR:HG23 | 17 | 0.66 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 20 | 0.66 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 15 | 0.66 |
| (4,300) | 1:97:A:LEU:HD23 | 1:175:A:PHE:HB3 | 17 | 0.66 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 10 | 0.66 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 11 | 0.66 |
| (4,192) | 1:176:A:ILE:HA | 1:110:A:LEU:HD13 | 18 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 11 | 0.66 |
| (4,70) | 1:130:A:THR:H | 2:201:A:NAD:H4D | 2 | 0.66 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 8 | 0.66 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD12 | 14 | 0.66 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 8 | 0.66 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 19 | 0.66 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 11 | 0.66 |
| (2,3784) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE3 | 3 | 0.66 |
| (2,3772) | 1:151:A:MET:HE3 | 1:174:A:GLU:HG2 | 7 | 0.66 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 15 | 0.66 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 2 | 0.66 |
| (2,3466) | 1:97:A:LEU:HD21 | 1:166:A:TRP:HB2 | 5 | 0.66 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 2 | 0.66 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 9 | 0.66 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 10 | 0.66 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 11 | 0.66 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 12 | 0.66 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 3 | 0.66 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 12 | 0.66 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 11 | 0.66 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 12 | 0.66 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD23 | 20 | 0.66 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 7 | 0.66 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 11 | 0.66 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 1 | 0.66 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 13 | 0.66 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 17 | 0.66 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 20 | 0.66 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD12 | 9 | 0.66 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 18 | 0.66 |
| (2,1831) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 7 | 0.66 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 10 | 0.66 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 13 | 0.66 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 20 | 0.66 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 6 | 0.66 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 9 | 0.66 |
| (2,1690) | 1:63:A:LYS:HG2 | 1:62:A:LYS:HA | 17 | 0.66 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 13 | 0.66 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 1 | 0.66 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 4 | 0.66 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 11 | 0.66 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 12 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 19 | 0.66 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 4 | 0.66 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 17 | 0.66 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 10 | 0.66 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 11 | 0.66 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 15 | 0.66 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 13 | 0.66 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 14 | 0.66 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 17 | 0.66 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 6 | 0.66 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 10 | 0.66 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 20 | 0.66 |
| (2,339) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 16 | 0.66 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 5 | 0.66 |
| (2,122) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 15 | 0.66 |
| (2,67) | 1:176:A:ILE:HG21 | 1:177:A:LYS:H | 20 | 0.66 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 13 | 0.65 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 15 | 0.65 |
| (4,292) | 1:122:A:VAL:HG21 | 1:118:A:SER:H | 5 | 0.65 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 19 | 0.65 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 2 | 0.65 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 18 | 0.65 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 17 | 0.65 |
| (4,166) | 1:171:A:VAL:H | 1:168:A:ILE:HG13 | 7 | 0.65 |
| (2,3813) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 1 | 0.65 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 10 | 0.65 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 16 | 0.65 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 4 | 0.65 |
| (2,3657) | 1:63:A:LYS:HG3 | 1:62:A:LYS:HA | 11 | 0.65 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 7 | 0.65 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 9 | 0.65 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 11 | 0.65 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 13 | 0.65 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 19 | 0.65 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 6 | 0.65 |
| (2,3466) | 1:97:A:LEU:HD22 | 1:166:A:TRP:HB2 | 18 | 0.65 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 11 | 0.65 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 3 | 0.65 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 5 | 0.65 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 13 | 0.65 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 15 | 0.65 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 20 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 10 | 0.65 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 18 | 0.65 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 3 | 0.65 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 4 | 0.65 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD23 | 9 | 0.65 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 16 | 0.65 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 13 | 0.65 |
| (2,2784) | 1:53:A:LEU:HD22 | 1:53:A:LEU:H | 16 | 0.65 |
| (2,1859) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 8 | 0.65 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 20 | 0.65 |
| (2,1847) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 9 | 0.65 |
| (2,1840) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG21 | 20 | 0.65 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 5 | 0.65 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 4 | 0.65 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 11 | 0.65 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG12 | 6 | 0.65 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 16 | 0.65 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 2 | 0.65 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 3 | 0.65 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 5 | 0.65 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 10 | 0.65 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 13 | 0.65 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 14 | 0.65 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 18 | 0.65 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 20 | 0.65 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 19 | 0.65 |
| (2,1473) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 19 | 0.65 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 5 | 0.65 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 4 | 0.65 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 17 | 0.65 |
| (2,1377) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 4 | 0.65 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 8 | 0.65 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 14 | 0.65 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 20 | 0.65 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 19 | 0.65 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 1 | 0.65 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 10 | 0.65 |
| (2,948) | 1:76:A:ALA:HB1 | 1:78:A:GLN:HE22 | 8 | 0.65 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 12 | 0.65 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 12 | 0.65 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 12 | 0.65 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 15 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 5 | 0.65 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 8 | 0.65 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 16 | 0.65 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 19 | 0.65 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 13 | 0.64 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 6 | 0.64 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 8 | 0.64 |
| (4,384) | 1:178:A:VAL:HA | 1:110:A:LEU:HD11 | 1 | 0.64 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 5 | 0.64 |
| (4,332) | 1:37:A:LEU:HD12 | 1:41:A:MET:HB2 | 9 | 0.64 |
| (4,325) | 1:7:A:VAL:HG13 | 1:10:A:PHE:HB3 | 20 | 0.64 |
| (4,311) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 5 | 0.64 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 11 | 0.64 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 16 | 0.64 |
| (4,299) | 1:168:A:ILE:HD12 | 1:152:A:ALA:HA | 18 | 0.64 |
| (4,278) | 1:142:A:VAL:HG12 | 1:102:A:ALA:H | 10 | 0.64 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 12 | 0.64 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 17 | 0.64 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 4 | 0.64 |
| (4,222) | 1:57:A:VAL:HG23 | 1:74:A:ILE:HB | 6 | 0.64 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 6 | 0.64 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 2 | 0.64 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 13 | 0.64 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 14 | 0.64 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 2 | 0.64 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 19 | 0.64 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 5 | 0.64 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 10 | 0.64 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 17 | 0.64 |
| (2,3466) | 1:97:A:LEU:HD22 | 1:166:A:TRP:HB2 | 8 | 0.64 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 7 | 0.64 |
| (2,3400) | 1:38:A:LEU:HD23 | 1:39:A:ALA:H | 8 | 0.64 |
| (2,3346) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 4 | 0.64 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 8 | 0.64 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 10 | 0.64 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 17 | 0.64 |
| (2,3265) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 8 | 0.64 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD21 | 3 | 0.64 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 15 | 0.64 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 1 | 0.64 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 2 | 0.64 |
| (2,1884) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 18 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG22 | 11 | 0.64 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 1 | 0.64 |
| (2,1823) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE1 | 20 | 0.64 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 14 | 0.64 |
| (2,1690) | 1:63:A:LYS:HG2 | 1:62:A:LYS:HA | 13 | 0.64 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 6 | 0.64 |
| (2,1601) | 1:41:A:MET:HE2 | 1:10:A:PHE:HB3 | 19 | 0.64 |
| (2,1566) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 14 | 0.64 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 6 | 0.64 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 7 | 0.64 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 8 | 0.64 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 9 | 0.64 |
| (2,1525) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 15 | 0.64 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 2 | 0.64 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 4 | 0.64 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 3 | 0.64 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 7 | 0.64 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 9 | 0.64 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 11 | 0.64 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 15 | 0.64 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 19 | 0.64 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 20 | 0.64 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 3 | 0.64 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 13 | 0.64 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 16 | 0.64 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 2 | 0.64 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 5 | 0.64 |
| (2,561) | 1:16:A:ARG:H | 1:16:A:ARG:HB2 | 20 | 0.64 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 20 | 0.64 |
| (2,342) | 1:41:A:MET:H | 1:41:A:MET:HG2 | 17 | 0.64 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 1 | 0.64 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 12 | 0.64 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 13 | 0.64 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 14 | 0.64 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 20 | 0.64 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 16 | 0.64 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG21 | 6 | 0.63 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 10 | 0.63 |
| (4,332) | 1:37:A:LEU:HD13 | 1:41:A:MET:HB2 | 2 | 0.63 |
| (4,332) | 1:37:A:LEU:HD11 | 1:41:A:MET:HB2 | 10 | 0.63 |
| (4,332) | 1:37:A:LEU:HD11 | 1:41:A:MET:HB2 | 11 | 0.63 |
| (4,332) | 1:37:A:LEU:HD11 | 1:41:A:MET:HB2 | 15 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,292) | 1:122:A:VAL:HG22 | 1:118:A:SER:H | 20 | 0.63 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 2 | 0.63 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 6 | 0.63 |
| (4,278) | 1:142:A:VAL:HG12 | 1:102:A:ALA:H | 7 | 0.63 |
| (4,227) | 1:8:A:SER:HB3 | 1:55:A:HIS:HD2 | 10 | 0.63 |
| (4,204) | 1:173:A:ALA:HB1 | 1:111:A:LYS:HG3 | 11 | 0.63 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB2 | 15 | 0.63 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD22 | 2 | 0.63 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 20 | 0.63 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 3 | 0.63 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE3 | 4 | 0.63 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 3 | 0.63 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 10 | 0.63 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 17 | 0.63 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 8 | 0.63 |
| (2,3466) | 1:97:A:LEU:HD22 | 1:166:A:TRP:HB2 | 15 | 0.63 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 7 | 0.63 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 8 | 0.63 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 11 | 0.63 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 14 | 0.63 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 15 | 0.63 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 20 | 0.63 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 14 | 0.63 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 4 | 0.63 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 8 | 0.63 |
| (2,2784) | 1:53:A:LEU:HD21 | 1:53:A:LEU:H | 2 | 0.63 |
| (2,2509) | 1:38:A:LEU:H | 1:38:A:LEU:HG | 16 | 0.63 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 12 | 0.63 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 3 | 0.63 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 4 | 0.63 |
| (2,1846) | 1:160:A:LEU:HD11 | 1:91:A:GLN:HB2 | 7 | 0.63 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 9 | 0.63 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 12 | 0.63 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 8 | 0.63 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 19 | 0.63 |
| (2,1808) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HG | 2 | 0.63 |
| (2,1565) | 1:22:A:ILE:HG22 | 1:41:A:MET:HB2 | 16 | 0.63 |
| (2,1529) | 1:144:A:LEU:HD22 | 1:145:A:SER:HB2 | 9 | 0.63 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 17 | 0.63 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 11 | 0.63 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 14 | 0.63 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 20 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1314) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 10 | 0.63 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 2 | 0.63 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 7 | 0.63 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 8 | 0.63 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 18 | 0.63 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 20 | 0.63 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 11 | 0.63 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 2 | 0.63 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 20 | 0.63 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 7 | 0.63 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 12 | 0.63 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 1 | 0.63 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 2 | 0.63 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 9 | 0.63 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 11 | 0.63 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HG3 | 5 | 0.62 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 2 | 0.62 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 10 | 0.62 |
| (4,311) | 1:143:A:VAL:HG12 | 1:178:A:VAL:HA | 12 | 0.62 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 8 | 0.62 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 7 | 0.62 |
| (4,203) | 1:173:A:ALA:HB2 | 1:171:A:VAL:HB | 16 | 0.62 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 13 | 0.62 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD21 | 5 | 0.62 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 7 | 0.62 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 12 | 0.62 |
| (2,3813) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 9 | 0.62 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 7 | 0.62 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE1 | 14 | 0.62 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 1 | 0.62 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 15 | 0.62 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 3 | 0.62 |
| (2,3532) | 1:21:A:LEU:HD13 | 1:41:A:MET:HB2 | 20 | 0.62 |
| (2,3514) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 2 | 0.62 |
| (2,3514) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 9 | 0.62 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 2 | 0.62 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 4 | 0.62 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 9 | 0.62 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 10 | 0.62 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 20 | 0.62 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 4 | 0.62 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 13 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3481) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 2 | 0.62 |
| (2,3378) | 1:66:A:ALA:HB2 | 1:31:A:TRP:HZ3 | 12 | 0.62 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 2 | 0.62 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 7 | 0.62 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 19 | 0.62 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 11 | 0.62 |
| (2,3265) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 10 | 0.62 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 1 | 0.62 |
| (2,2308) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 18 | 0.62 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 5 | 0.62 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 8 | 0.62 |
| (2,1884) | 1:41:A:MET:HE3 | 1:46:A:HIS:HA | 20 | 0.62 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG23 | 12 | 0.62 |
| (2,1840) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG21 | 6 | 0.62 |
| (2,1840) | 1:128:A:ILE:HG23 | 1:129:A:THR:HG21 | 12 | 0.62 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 1 | 0.62 |
| (2,1831) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 6 | 0.62 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 3 | 0.62 |
| (2,1742) | 1:110:A:LEU:HD12 | 1:173:A:ALA:HA | 3 | 0.62 |
| (2,1690) | 1:63:A:LYS:HG3 | 1:62:A:LYS:HA | 19 | 0.62 |
| (2,1554) | 1:38:A:LEU:HD21 | 1:50:A:MET:HG2 | 9 | 0.62 |
| (2,1511) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 2 | 0.62 |
| (2,1490) | 1:167:A:LEU:HD12 | 1:166:A:TRP:HA | 6 | 0.62 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 6 | 0.62 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 9 | 0.62 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 6 | 0.62 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 2 | 0.62 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 8 | 0.62 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 15 | 0.62 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 7 | 0.62 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 11 | 0.62 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 9 | 0.62 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 4 | 0.62 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 6 | 0.62 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 9 | 0.61 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 20 | 0.61 |
| (4,449) | 1:74:A:ILE:HD12 | 1:11:A:LEU:HD23 | 2 | 0.61 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 7 | 0.61 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 14 | 0.61 |
| (4,415) | 1:19:A:PRO:HB2 | 1:36:A:GLU:HG2 | 12 | 0.61 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 18 | 0.61 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 15 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,204) | 1:173:A:ALA:HB2 | 1:111:A:LYS:HG2 | 8 | 0.61 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 7 | 0.61 |
| (2,3964) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H6N | 9 | 0.61 |
| (2,3813) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 7 | 0.61 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 2 | 0.61 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 6 | 0.61 |
| (2,3784) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 15 | 0.61 |
| (2,3722) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 9 | 0.61 |
| (2,3722) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 14 | 0.61 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 5 | 0.61 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 5 | 0.61 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 6 | 0.61 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 13 | 0.61 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 1 | 0.61 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 20 | 0.61 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 12 | 0.61 |
| (2,3428) | 1:108:A:LEU:HD12 | 2:201:A:NAD:H2A | 19 | 0.61 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 6 | 0.61 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 9 | 0.61 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 5 | 0.61 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 18 | 0.61 |
| (2,3265) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 9 | 0.61 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 3 | 0.61 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 12 | 0.61 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 18 | 0.61 |
| (2,1875) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 6 | 0.61 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD12 | 4 | 0.61 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 14 | 0.61 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 12 | 0.61 |
| (2,1840) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG22 | 2 | 0.61 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 3 | 0.61 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 7 | 0.61 |
| (2,1827) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HG | 1 | 0.61 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 6 | 0.61 |
| (2,1823) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 2 | 0.61 |
| (2,1808) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HG | 8 | 0.61 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 9 | 0.61 |
| (2,1808) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HG | 11 | 0.61 |
| (2,1808) | 1:13:A:LEU:HD22 | 1:13:A:LEU:HG | 13 | 0.61 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 10 | 0.61 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 13 | 0.61 |
| (2,1425) | 1:56:A:ILE:HG21 | 1:65:A:PHE:HD1 | 14 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 8 | 0.61 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 13 | 0.61 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 9 | 0.61 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 16 | 0.61 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 7 | 0.61 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 20 | 0.61 |
| (2,954) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 10 | 0.61 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 14 | 0.61 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 15 | 0.61 |
| (2,339) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 2 | 0.61 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 11 | 0.61 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 18 | 0.61 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 6 | 0.61 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 18 | 0.61 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 12 | 0.6 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 18 | 0.6 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 14 | 0.6 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 20 | 0.6 |
| (4,278) | 1:142:A:VAL:HG12 | 1:102:A:ALA:H | 11 | 0.6 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 10 | 0.6 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 10 | 0.6 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 17 | 0.6 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 4 | 0.6 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 13 | 0.6 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD21 | 6 | 0.6 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD23 | 19 | 0.6 |
| (2,3839) | 1:129:A:THR:HG21 | 1:129:A:THR:HA | 6 | 0.6 |
| (2,3813) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD13 | 6 | 0.6 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 3 | 0.6 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 13 | 0.6 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 2 | 0.6 |
| (2,3722) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 6 | 0.6 |
| (2,3600) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 3 | 0.6 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 8 | 0.6 |
| (2,3532) | 1:21:A:LEU:HD12 | 1:41:A:MET:HB2 | 5 | 0.6 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 4 | 0.6 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 1 | 0.6 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 7 | 0.6 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 11 | 0.6 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 12 | 0.6 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 16 | 0.6 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 18 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 6 | 0.6 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 9 | 0.6 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 19 | 0.6 |
| (2,3462) | 1:168:A:ILE:HD11 | 1:175:A:PHE:HB3 | 13 | 0.6 |
| (2,3416) | 1:143:A:VAL:HG12 | 1:143:A:VAL:H | 18 | 0.6 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 16 | 0.6 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 15 | 0.6 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 1 | 0.6 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG22 | 16 | 0.6 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG23 | 4 | 0.6 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 1 | 0.6 |
| (2,1831) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 5 | 0.6 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 9 | 0.6 |
| (2,1823) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE3 | 3 | 0.6 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 10 | 0.6 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 13 | 0.6 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 5 | 0.6 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 7 | 0.6 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 10 | 0.6 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 15 | 0.6 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 19 | 0.6 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 3 | 0.6 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 16 | 0.6 |
| (2,1495) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 8 | 0.6 |
| (2,1490) | 1:167:A:LEU:HD12 | 1:166:A:TRP:HA | 5 | 0.6 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 1 | 0.6 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 2 | 0.6 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 6 | 0.6 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 12 | 0.6 |
| (2,1297) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 17 | 0.6 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 1 | 0.6 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 7 | 0.6 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 7 | 0.6 |
| (2,602) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 19 | 0.6 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 4 | 0.6 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 18 | 0.6 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 12 | 0.6 |
| (2,305) | 1:42:A:LYS:HA | 1:46:A:HIS:H | 14 | 0.6 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 2 | 0.6 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 7 | 0.6 |
| (2,110) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 10 | 0.6 |
| (4,449) | 1:74:A:ILE:HD12 | 1:11:A:LEU:HD23 | 7 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,449) | 1:74:A:ILE:HD11 | 1:57:A:VAL:HG23 | 13 | 0.59 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 4 | 0.59 |
| (4,410) | 1:50:A:MET:HE3 | 1:54:A:LYS:HD2 | 5 | 0.59 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 17 | 0.59 |
| (4,329) | 1:142:A:VAL:HG21 | 1:103:A:GLU:HA | 4 | 0.59 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 2 | 0.59 |
| (4,292) | 1:122:A:VAL:HG21 | 1:118:A:SER:H | 8 | 0.59 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 1 | 0.59 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 4 | 0.59 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 2 | 0.59 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD11 | 5 | 0.59 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD21 | 11 | 0.59 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD23 | 13 | 0.59 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 11 | 0.59 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 20 | 0.59 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 3 | 0.59 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 15 | 0.59 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 2 | 0.59 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 10 | 0.59 |
| (2,3470) | 1:110:A:LEU:HD12 | 1:107:A:ASP:HA | 15 | 0.59 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 12 | 0.59 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 16 | 0.59 |
| (2,3265) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 12 | 0.59 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD21 | 2 | 0.59 |
| (2,1974) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 7 | 0.59 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 20 | 0.59 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 19 | 0.59 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE1 | 10 | 0.59 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 17 | 0.59 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB3 | 19 | 0.59 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 12 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 3 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 4 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 6 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 7 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 16 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 17 | 0.59 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 18 | 0.59 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 18 | 0.59 |
| (2,1783) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 1 | 0.59 |
| (2,1724) | 1:149:A:LYS:HA | 1:96:A:VAL:HG11 | 5 | 0.59 |
| (2,1601) | 1:41:A:MET:HE2 | 1:10:A:PHE:HB3 | 9 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1492) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 4 | 0.59 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 7 | 0.59 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 13 | 0.59 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 19 | 0.59 |
| (2,1462) | 1:14:A:VAL:HG23 | 1:14:A:VAL:H | 13 | 0.59 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 2 | 0.59 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 8 | 0.59 |
| (2,1388) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 20 | 0.59 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 7 | 0.59 |
| (2,948) | 1:76:A:ALA:HB3 | 1:78:A:GLN:HE22 | 15 | 0.59 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 12 | 0.59 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 9 | 0.59 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 11 | 0.59 |
| (2,305) | 1:42:A:LYS:HA | 1:46:A:HIS:H | 16 | 0.59 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 10 | 0.59 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 18 | 0.59 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG21 | 9 | 0.58 |
| (4,437) | 1:178:A:VAL:HG23 | 1:177:A:LYS:HG2 | 3 | 0.58 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 20 | 0.58 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD11 | 4 | 0.58 |
| (4,368) | 1:20:A:ALA:HB1 | 1:22:A:ILE:HB | 13 | 0.58 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 11 | 0.58 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 10 | 0.58 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 19 | 0.58 |
| (4,332) | 1:37:A:LEU:HD11 | 1:41:A:MET:HB2 | 12 | 0.58 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 6 | 0.58 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 9 | 0.58 |
| (4,15) | 1:177:A:LYS:H | 1:96:A:VAL:HG21 | 3 | 0.58 |
| (4,12) | 1:175:A:PHE:HE1 | 1:168:A:ILE:HG23 | 2 | 0.58 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD22 | 7 | 0.58 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 15 | 0.58 |
| (2,3784) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE3 | 11 | 0.58 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 7 | 0.58 |
| (2,3657) | 1:63:A:LYS:HG3 | 1:62:A:LYS:HA | 9 | 0.58 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 7 | 0.58 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 18 | 0.58 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 8 | 0.58 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 14 | 0.58 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 7 | 0.58 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 18 | 0.58 |
| (2,3470) | 1:110:A:LEU:HD13 | 1:107:A:ASP:HA | 9 | 0.58 |
| (2,3459) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 5 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3415) | 1:122:A:VAL:HG21 | 1:122:A:VAL:H | 5 | 0.58 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 15 | 0.58 |
| (2,3271) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HB3 | 17 | 0.58 |
| (2,2784) | 1:53:A:LEU:HD23 | 1:53:A:LEU:H | 15 | 0.58 |
| (2,1974) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 13 | 0.58 |
| (2,1851) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 2 | 0.58 |
| (2,1835) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 5 | 0.58 |
| (2,1831) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 13 | 0.58 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 2 | 0.58 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 20 | 0.58 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 1 | 0.58 |
| (2,1808) | 1:13:A:LEU:HD23 | 1:13:A:LEU:HG | 12 | 0.58 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 14 | 0.58 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 20 | 0.58 |
| (2,1794) | 1:117:A:MET:HE1 | 1:117:A:MET:HB2 | 20 | 0.58 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 12 | 0.58 |
| (2,1690) | 1:63:A:LYS:HG3 | 1:62:A:LYS:HA | 11 | 0.58 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 17 | 0.58 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 1 | 0.58 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 9 | 0.58 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 10 | 0.58 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 15 | 0.58 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 16 | 0.58 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 19 | 0.58 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 2 | 0.58 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 10 | 0.58 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 18 | 0.58 |
| (2,1276) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HE1 | 2 | 0.58 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 3 | 0.58 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 17 | 0.58 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 9 | 0.58 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 19 | 0.58 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 6 | 0.58 |
| (4,332) | 1:37:A:LEU:HD12 | 1:41:A:MET:HB2 | 1 | 0.57 |
| (4,332) | 1:37:A:LEU:HD12 | 1:41:A:MET:HB2 | 3 | 0.57 |
| (4,332) | 1:37:A:LEU:HD11 | 1:41:A:MET:HB2 | 14 | 0.57 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 16 | 0.57 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 17 | 0.57 |
| (4,223) | 1:13:A:LEU:HD12 | 1:10:A:PHE:HE1 | 5 | 0.57 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 7 | 0.57 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 13 | 0.57 |
| (4,184) | 1:105:A:ASN:H | 1:136:A:MET:H | 18 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 11 | 0.57 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 13 | 0.57 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 14 | 0.57 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 3 | 0.57 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 11 | 0.57 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 11 | 0.57 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 12 | 0.57 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 20 | 0.57 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 17 | 0.57 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 3 | 0.57 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 14 | 0.57 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 16 | 0.57 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 4 | 0.57 |
| (2,3435) | 1:14:A:VAL:HG13 | 1:10:A:PHE:HD1 | 5 | 0.57 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 18 | 0.57 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 1 | 0.57 |
| (2,3182) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 5 | 0.57 |
| (2,3177) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 13 | 0.57 |
| (2,2308) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 19 | 0.57 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 20 | 0.57 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 5 | 0.57 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 17 | 0.57 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 18 | 0.57 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 11 | 0.57 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 18 | 0.57 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 12 | 0.57 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE3 | 4 | 0.57 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 18 | 0.57 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 2 | 0.57 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 12 | 0.57 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 8 | 0.57 |
| (2,1492) | 1:167:A:LEU:HD21 | 1:123:A:HIS:HA | 20 | 0.57 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 4 | 0.57 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 5 | 0.57 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 8 | 0.57 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 12 | 0.57 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 17 | 0.57 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 8 | 0.57 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 14 | 0.57 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 18 | 0.57 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 3 | 0.57 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 10 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 16 | 0.57 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 18 | 0.57 |
| (2,339) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 8 | 0.57 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 12 | 0.57 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 17 | 0.57 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 20 | 0.57 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HG3 | 2 | 0.56 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 12 | 0.56 |
| (4,449) | 1:57:A:VAL:HG21 | 1:74:A:ILE:HD11 | 4 | 0.56 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 1 | 0.56 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 13 | 0.56 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 18 | 0.56 |
| (4,328) | 1:122:A:VAL:HG13 | 1:113:A:GLY:HA2 | 13 | 0.56 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 17 | 0.56 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 8 | 0.56 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 18 | 0.56 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 3 | 0.56 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 3 | 0.56 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 7 | 0.56 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 15 | 0.56 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD3 | 14 | 0.56 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 19 | 0.56 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 2 | 0.56 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 8 | 0.56 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD23 | 16 | 0.56 |
| (2,3843) | 1:76:A:ALA:HB3 | 1:16:A:ARG:HA | 15 | 0.56 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD11 | 13 | 0.56 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 10 | 0.56 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 9 | 0.56 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 4 | 0.56 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 1 | 0.56 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 12 | 0.56 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 20 | 0.56 |
| (2,3470) | 1:110:A:LEU:HD13 | 1:107:A:ASP:HA | 14 | 0.56 |
| (2,3415) | 1:122:A:VAL:HG22 | 1:122:A:VAL:H | 7 | 0.56 |
| (2,3415) | 1:122:A:VAL:HG22 | 1:122:A:VAL:H | 17 | 0.56 |
| (2,3265) | 1:84:A:VAL:HG13 | 1:84:A:VAL:H | 3 | 0.56 |
| (2,2266) | 1:153:A:ASP:H | 1:95:A:ALA:HB1 | 6 | 0.56 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 14 | 0.56 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 5 | 0.56 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG23 | 19 | 0.56 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 13 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 7 | 0.56 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 8 | 0.56 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 9 | 0.56 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD13 | 11 | 0.56 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 15 | 0.56 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 20 | 0.56 |
| (2,1813) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HG | 12 | 0.56 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 19 | 0.56 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 16 | 0.56 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 18 | 0.56 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 18 | 0.56 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 2 | 0.56 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 6 | 0.56 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 7 | 0.56 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 14 | 0.56 |
| (2,1391) | 1:56:A:ILE:HB | 1:57:A:VAL:H | 5 | 0.56 |
| (2,1276) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HE1 | 10 | 0.56 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 20 | 0.56 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 17 | 0.56 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 14 | 0.56 |
| (2,948) | 1:76:A:ALA:HB3 | 1:78:A:GLN:HE22 | 2 | 0.56 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 4 | 0.56 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 6 | 0.56 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 1 | 0.56 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 14 | 0.56 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 14 | 0.56 |
| (2,305) | 1:42:A:LYS:HA | 1:46:A:HIS:H | 17 | 0.56 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 10 | 0.56 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 14 | 0.56 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 11 | 0.56 |
| (4,449) | 1:74:A:ILE:HD11 | 1:57:A:VAL:HG23 | 1 | 0.55 |
| (4,449) | 1:74:A:ILE:HD12 | 1:11:A:LEU:HD21 | 8 | 0.55 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 1 | 0.55 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 12 | 0.55 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 2 | 0.55 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 6 | 0.55 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD3 | 17 | 0.55 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 14 | 0.55 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 14 | 0.55 |
| (4,6) | 1:65:A:PHE:HE1 | 1:74:A:ILE:HG23 | 4 | 0.55 |
| (2,3839) | 1:129:A:THR:HG21 | 1:129:A:THR:HA | 20 | 0.55 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 1 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 13 | 0.55 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 5 | 0.55 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD11 | 7 | 0.55 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 16 | 0.55 |
| (2,3772) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 16 | 0.55 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 19 | 0.55 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 7 | 0.55 |
| (2,3570) | 1:4:A:MET:HE3 | 1:52:A:GLU:HA | 1 | 0.55 |
| (2,3570) | 1:4:A:MET:HE2 | 1:52:A:GLU:HA | 18 | 0.55 |
| (2,3454) | 1:168:A:ILE:HD13 | 1:149:A:LYS:H | 5 | 0.55 |
| (2,3446) | 1:74:A:ILE:HD12 | 1:67:A:PHE:HE1 | 5 | 0.55 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 5 | 0.55 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 6 | 0.55 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 7 | 0.55 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 10 | 0.55 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 13 | 0.55 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 15 | 0.55 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 19 | 0.55 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 3 | 0.55 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 5 | 0.55 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 10 | 0.55 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 12 | 0.55 |
| (2,1823) | 1:37:A:LEU:HD11 | 1:41:A:MET:HE1 | 15 | 0.55 |
| (2,1819) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HG | 13 | 0.55 |
| (2,1813) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HG | 8 | 0.55 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 14 | 0.55 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 16 | 0.55 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 20 | 0.55 |
| (2,1808) | 1:13:A:LEU:HD21 | 1:13:A:LEU:HG | 5 | 0.55 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 2 | 0.55 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 20 | 0.55 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 3 | 0.55 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 11 | 0.55 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 18 | 0.55 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 5 | 0.55 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 19 | 0.55 |
| (2,1314) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 3 | 0.55 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 1 | 0.55 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 15 | 0.55 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 18 | 0.55 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 5 | 0.55 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 12 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 4 | 0.54 |
| (4,449) | 1:57:A:VAL:HG21 | 1:74:A:ILE:HD11 | 16 | 0.54 |
| (4,449) | 1:74:A:ILE:HD11 | 1:57:A:VAL:HG23 | 20 | 0.54 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 17 | 0.54 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 9 | 0.54 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 4 | 0.54 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 6 | 0.54 |
| (4,368) | 1:20:A:ALA:HB1 | 1:22:A:ILE:HB | 12 | 0.54 |
| (4,338) | 1:111:A:LYS:HD3 | 1:104:A:LYS:HA | 3 | 0.54 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 4 | 0.54 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 12 | 0.54 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD11 | 1 | 0.54 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD11 | 7 | 0.54 |
| (4,15) | 1:177:A:LYS:H | 1:96:A:VAL:HG21 | 16 | 0.54 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 14 | 0.54 |
| (2,3788) | 1:151:A:MET:HE1 | 1:151:A:MET:HG3 | 20 | 0.54 |
| (2,3784) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE3 | 19 | 0.54 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 6 | 0.54 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 7 | 0.54 |
| (2,3514) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 12 | 0.54 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 11 | 0.54 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 7 | 0.54 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 4 | 0.54 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 14 | 0.54 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 8 | 0.54 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 9 | 0.54 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 11 | 0.54 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 12 | 0.54 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 16 | 0.54 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 20 | 0.54 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 14 | 0.54 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 20 | 0.54 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 13 | 0.54 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 14 | 0.54 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 18 | 0.54 |
| (2,1820) | 1:142:A:VAL:HG11 | 1:142:A:VAL:HB | 2 | 0.54 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 20 | 0.54 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 10 | 0.54 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 4 | 0.54 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 7 | 0.54 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 9 | 0.54 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 11 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 13 | 0.54 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 14 | 0.54 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 14 | 0.54 |
| (2,1601) | 1:41:A:MET:HE2 | 1:10:A:PHE:HB3 | 11 | 0.54 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 18 | 0.54 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 18 | 0.54 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 8 | 0.54 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 17 | 0.54 |
| (2,539) | 1:38:A:LEU:H | 1:37:A:LEU:HB3 | 1 | 0.54 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 7 | 0.54 |
| (2,16) | 1:21:A:LEU:HD13 | 1:10:A:PHE:HE1 | 7 | 0.54 |
| (4,449) | 1:74:A:ILE:HD11 | 1:57:A:VAL:HG23 | 19 | 0.53 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 17 | 0.53 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 5 | 0.53 |
| (4,368) | 1:20:A:ALA:HB1 | 1:22:A:ILE:HB | 11 | 0.53 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 16 | 0.53 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 10 | 0.53 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 1 | 0.53 |
| (4,184) | 1:64:A:ARG:H | 1:12:A:SER:H | 2 | 0.53 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 17 | 0.53 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB2 | 6 | 0.53 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 7 | 0.53 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 11 | 0.53 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 8 | 0.53 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD22 | 9 | 0.53 |
| (2,3839) | 1:129:A:THR:HG22 | 1:129:A:THR:HA | 2 | 0.53 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD12 | 12 | 0.53 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 14 | 0.53 |
| (2,3784) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE3 | 13 | 0.53 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 15 | 0.53 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 6 | 0.53 |
| (2,3508) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 12 | 0.53 |
| (2,3507) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 20 | 0.53 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 15 | 0.53 |
| (2,3470) | 1:110:A:LEU:HD13 | 1:107:A:ASP:HA | 5 | 0.53 |
| (2,3461) | 1:168:A:ILE:HD12 | 1:156:A:PHE:HB2 | 17 | 0.53 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 1 | 0.53 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 17 | 0.53 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 1 | 0.53 |
| (2,3270) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 20 | 0.53 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 4 | 0.53 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 6 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 11 | 0.53 |
| (2,1814) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HB | 16 | 0.53 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 8 | 0.53 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 1 | 0.53 |
| (2,1794) | 1:117:A:MET:HE1 | 1:117:A:MET:HB2 | 17 | 0.53 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 3 | 0.53 |
| (2,1607) | 1:73:A:LYS:HD2 | 1:33:A:PRO:HB2 | 20 | 0.53 |
| (2,1490) | 1:167:A:LEU:HD12 | 1:166:A:TRP:HA | 2 | 0.53 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 4 | 0.53 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 11 | 0.53 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 10 | 0.53 |
| (2,1276) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HE1 | 9 | 0.53 |
| (2,1276) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HE1 | 19 | 0.53 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 13 | 0.53 |
| (2,980) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 19 | 0.53 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 3 | 0.53 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 12 | 0.53 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 6 | 0.53 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 7 | 0.53 |
| (2,339) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 11 | 0.53 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 8 | 0.53 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 4 | 0.53 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 10 | 0.53 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 19 | 0.52 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD21 | 14 | 0.52 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG23 | 3 | 0.52 |
| (4,449) | 1:74:A:ILE:HD11 | 1:11:A:LEU:HD21 | 5 | 0.52 |
| (4,449) | 1:74:A:ILE:HD11 | 1:11:A:LEU:HD21 | 14 | 0.52 |
| (4,409) | 1:4:A:MET:HE3 | 1:59:A:THR:HG23 | 18 | 0.52 |
| (4,353) | 1:165:A:VAL:HB | 1:131:A:ALA:HA | 17 | 0.52 |
| (4,352) | 1:36:A:GLU:HB3 | 1:42:A:LYS:HE3 | 7 | 0.52 |
| (4,320) | 1:151:A:MET:HE2 | 1:147:A:ASP:HB2 | 17 | 0.52 |
| (4,303) | 1:110:A:LEU:HD12 | 1:107:A:ASP:HA | 15 | 0.52 |
| (4,301) | 1:97:A:LEU:HD23 | 1:156:A:PHE:HB2 | 9 | 0.52 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 10 | 0.52 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 11 | 0.52 |
| (4,278) | 1:142:A:VAL:HG12 | 1:102:A:ALA:H | 4 | 0.52 |
| (4,259) | 1:117:A:MET:HE3 | 2:201:A:NAD:H2A | 17 | 0.52 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 16 | 0.52 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 18 | 0.52 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 1 | 0.52 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 9 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,129) | 1:13:A:LEU:HD21 | 1:18:A:ASN:H | 5 | 0.52 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 3 | 0.52 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 10 | 0.52 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 3 | 0.52 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 9 | 0.52 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 17 | 0.52 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 5 | 0.52 |
| (2,3832) | 1:97:A:LEU:HD22 | 1:151:A:MET:HG3 | 2 | 0.52 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 8 | 0.52 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 14 | 0.52 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 20 | 0.52 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 11 | 0.52 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 14 | 0.52 |
| (2,3527) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 4 | 0.52 |
| (2,3409) | 1:84:A:VAL:HG11 | 1:85:A:ASP:H | 5 | 0.52 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 2 | 0.52 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 3 | 0.52 |
| (2,1884) | 1:41:A:MET:HE3 | 1:46:A:HIS:HA | 17 | 0.52 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 6 | 0.52 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 19 | 0.52 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 8 | 0.52 |
| (2,1849) | 1:15:A:LEU:HD11 | 1:74:A:ILE:HD12 | 17 | 0.52 |
| (2,1823) | 1:37:A:LEU:HD12 | 1:41:A:MET:HE3 | 11 | 0.52 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 2 | 0.52 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 3 | 0.52 |
| (2,1813) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HG | 17 | 0.52 |
| (2,1793) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HB2 | 6 | 0.52 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG21 | 16 | 0.52 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 14 | 0.52 |
| (2,1555) | 1:84:A:VAL:HG21 | 1:85:A:ASP:HB2 | 2 | 0.52 |
| (2,1490) | 1:167:A:LEU:HD13 | 1:166:A:TRP:HA | 10 | 0.52 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 8 | 0.52 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 7 | 0.52 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 18 | 0.52 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 13 | 0.52 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD22 | 5 | 0.52 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 19 | 0.52 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 3 | 0.52 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 6 | 0.52 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG21 | 10 | 0.51 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG21 | 18 | 0.51 |
| (4,446) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HG | 6 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD11 | 4 | 0.51 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 11 | 0.51 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 14 | 0.51 |
| (4,379) | 1:50:A:MET:HA | 1:39:A:ALA:HB3 | 7 | 0.51 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 12 | 0.51 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 13 | 0.51 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 3 | 0.51 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 7 | 0.51 |
| (4,338) | 1:111:A:LYS:HD3 | 1:104:A:LYS:HA | 6 | 0.51 |
| (4,338) | 1:111:A:LYS:HD3 | 1:104:A:LYS:HA | 18 | 0.51 |
| (4,303) | 1:110:A:LEU:HD13 | 1:107:A:ASP:HA | 9 | 0.51 |
| (4,300) | 1:97:A:LEU:HD23 | 1:156:A:PHE:HB3 | 16 | 0.51 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 16 | 0.51 |
| (4,39) | 1:24:A:LEU:H | 1:17:A:HIS:HB2 | 16 | 0.51 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 16 | 0.51 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD22 | 8 | 0.51 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 18 | 0.51 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 11 | 0.51 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 16 | 0.51 |
| (2,3847) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 12 | 0.51 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD12 | 5 | 0.51 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 11 | 0.51 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD22 | 2 | 0.51 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 11 | 0.51 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 13 | 0.51 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 16 | 0.51 |
| (2,3788) | 1:151:A:MET:HE2 | 1:151:A:MET:HG3 | 5 | 0.51 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 6 | 0.51 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 9 | 0.51 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 9 | 0.51 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 12 | 0.51 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 8 | 0.51 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 13 | 0.51 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 2 | 0.51 |
| (2,3537) | 1:96:A:VAL:HG11 | 1:151:A:MET:HA | 14 | 0.51 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 13 | 0.51 |
| (2,3462) | 1:168:A:ILE:HD12 | 1:175:A:PHE:HB3 | 8 | 0.51 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 2 | 0.51 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 19 | 0.51 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 12 | 0.51 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 13 | 0.51 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 6 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 16 | 0.51 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 6 | 0.51 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 17 | 0.51 |
| (2,2823) | 1:74:A:ILE:H | 1:37:A:LEU:HD22 | 5 | 0.51 |
| (2,1877) | 1:129:A:THR:HG21 | 1:129:A:THR:HA | 6 | 0.51 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 10 | 0.51 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 16 | 0.51 |
| (2,1834) | 1:14:A:VAL:HG22 | 1:21:A:LEU:HG | 20 | 0.51 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 1 | 0.51 |
| (2,1824) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 16 | 0.51 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 5 | 0.51 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 16 | 0.51 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 19 | 0.51 |
| (2,1819) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HG | 20 | 0.51 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 1 | 0.51 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 15 | 0.51 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 18 | 0.51 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 3 | 0.51 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 13 | 0.51 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 7 | 0.51 |
| (2,1690) | 1:63:A:LYS:HG3 | 1:62:A:LYS:HA | 9 | 0.51 |
| (2,1541) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 2 | 0.51 |
| (2,1541) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 9 | 0.51 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 12 | 0.51 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 19 | 0.51 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 8 | 0.51 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 6 | 0.51 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 12 | 0.51 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 17 | 0.51 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 2 | 0.51 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 4 | 0.51 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 18 | 0.51 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 9 | 0.51 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 19 | 0.51 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB2 | 12 | 0.51 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD12 | 6 | 0.51 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 6 | 0.51 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 13 | 0.51 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 3 | 0.51 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 9 | 0.51 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 13 | 0.5 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG23 | 15 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,449) | 1:74:A:ILE:HD11 | 1:57:A:VAL:HG23 | 17 | 0.5 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 6 | 0.5 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 18 | 0.5 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 10 | 0.5 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 8 | 0.5 |
| (4,338) | 1:111:A:LYS:HD3 | 1:104:A:LYS:HA | 2 | 0.5 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 4 | 0.5 |
| (4,303) | 1:110:A:LEU:HD13 | 1:107:A:ASP:HA | 14 | 0.5 |
| (4,292) | 1:122:A:VAL:HG22 | 1:118:A:SER:H | 15 | 0.5 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 12 | 0.5 |
| (4,202) | 1:173:A:ALA:HA | 1:150:A:GLY:HA3 | 11 | 0.5 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 19 | 0.5 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 4 | 0.5 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 17 | 0.5 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 4 | 0.5 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD23 | 14 | 0.5 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 8 | 0.5 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 14 | 0.5 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 2 | 0.5 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 6 | 0.5 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 8 | 0.5 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 15 | 0.5 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 16 | 0.5 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 19 | 0.5 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 3 | 0.5 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 16 | 0.5 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD11 | 1 | 0.5 |
| (2,3784) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE1 | 9 | 0.5 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 11 | 0.5 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 11 | 0.5 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 17 | 0.5 |
| (2,3676) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 13 | 0.5 |
| (2,3676) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 18 | 0.5 |
| (2,3514) | 1:143:A:VAL:HG13 | 1:132:A:ARG:HA | 20 | 0.5 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 2 | 0.5 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 9 | 0.5 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 18 | 0.5 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 8 | 0.5 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 20 | 0.5 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 7 | 0.5 |
| (2,1897) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 1 | 0.5 |
| (2,1884) | 1:41:A:MET:HE3 | 1:46:A:HIS:HA | 16 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1874) | 1:168:A:ILE:HD12 | 1:171:A:VAL:HG13 | 5 | 0.5 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 15 | 0.5 |
| (2,1871) | 1:97:A:LEU:HD22 | 1:151:A:MET:HG3 | 5 | 0.5 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 2 | 0.5 |
| (2,1849) | 1:15:A:LEU:HD13 | 1:74:A:ILE:HD11 | 12 | 0.5 |
| (2,1846) | 1:160:A:LEU:HD13 | 1:91:A:GLN:HB2 | 18 | 0.5 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 5 | 0.5 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 14 | 0.5 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 10 | 0.5 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 15 | 0.5 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 16 | 0.5 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 4 | 0.5 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 1 | 0.5 |
| (2,1820) | 1:142:A:VAL:HG11 | 1:142:A:VAL:HB | 3 | 0.5 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 6 | 0.5 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 17 | 0.5 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 3 | 0.5 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 15 | 0.5 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 10 | 0.5 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 13 | 0.5 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 5 | 0.5 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 15 | 0.5 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 6 | 0.5 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 18 | 0.5 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 18 | 0.5 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 17 | 0.5 |
| (2,1490) | 1:167:A:LEU:HD12 | 1:166:A:TRP:HA | 18 | 0.5 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 1 | 0.5 |
| (2,1462) | 1:14:A:VAL:HG22 | 1:14:A:VAL:H | 20 | 0.5 |
| (2,1459) | 1:108:A:LEU:HD12 | 2:201:A:NAD:H2A | 19 | 0.5 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 13 | 0.5 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 14 | 0.5 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 12 | 0.5 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 2 | 0.5 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 9 | 0.5 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 1 | 0.5 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 2 | 0.5 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 14 | 0.5 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 11 | 0.5 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 4 | 0.5 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 7 | 0.5 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 5 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,187) | 1:26:A:LEU:HD23 | 1:26:A:LEU:H | 19 | 0.5 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 13 | 0.5 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 8 | 0.5 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 19 | 0.5 |
| (2,29) | 1:88:A:TYR:HD1 | 1:159:A:TYR:HD1 | 16 | 0.5 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD21 | 11 | 0.49 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG23 | 11 | 0.49 |
| (4,446) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HG | 2 | 0.49 |
| (4,446) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HG | 14 | 0.49 |
| (4,446) | 1:110:A:LEU:HD13 | 1:110:A:LEU:HG | 15 | 0.49 |
| (4,446) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HG | 18 | 0.49 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 10 | 0.49 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 18 | 0.49 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD11 | 3 | 0.49 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 10 | 0.49 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 13 | 0.49 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 10 | 0.49 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 2 | 0.49 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 5 | 0.49 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 7 | 0.49 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 1 | 0.49 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 6 | 0.49 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 2 | 0.49 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 15 | 0.49 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 4 | 0.49 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 9 | 0.49 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 18 | 0.49 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD12 | 9 | 0.49 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 6 | 0.49 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 13 | 0.49 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 18 | 0.49 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 9 | 0.49 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 18 | 0.49 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD21 | 1 | 0.49 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 16 | 0.49 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 12 | 0.49 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 17 | 0.49 |
| (2,3600) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 13 | 0.49 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 3 | 0.49 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 11 | 0.49 |
| (2,3466) | 1:97:A:LEU:HD22 | 1:166:A:TRP:HB2 | 17 | 0.49 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 20 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 4 | 0.49 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 10 | 0.49 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 17 | 0.49 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 4 | 0.49 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 6 | 0.49 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 10 | 0.49 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 11 | 0.49 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 5 | 0.49 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 8 | 0.49 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 9 | 0.49 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 11 | 0.49 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 16 | 0.49 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 9 | 0.49 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 6 | 0.49 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 19 | 0.49 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 19 | 0.49 |
| (2,1872) | 1:168:A:ILE:HD11 | 1:168:A:ILE:HG13 | 12 | 0.49 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 20 | 0.49 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 17 | 0.49 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 15 | 0.49 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 9 | 0.49 |
| (2,1840) | 1:128:A:ILE:HG23 | 1:129:A:THR:HG21 | 10 | 0.49 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 19 | 0.49 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 14 | 0.49 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 14 | 0.49 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 5 | 0.49 |
| (2,1807) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 15 | 0.49 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 7 | 0.49 |
| (2,1793) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HB2 | 18 | 0.49 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 17 | 0.49 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 19 | 0.49 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 1 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 2 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 6 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 8 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 9 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 10 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 12 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 13 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 16 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 17 | 0.49 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 18 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 20 | 0.49 |
| (2,1531) | 1:21:A:LEU:HD11 | 1:14:A:VAL:HA | 3 | 0.49 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 2 | 0.49 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 10 | 0.49 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 20 | 0.49 |
| (2,1462) | 1:14:A:VAL:HG21 | 1:14:A:VAL:H | 3 | 0.49 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 3 | 0.49 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 10 | 0.49 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 12 | 0.49 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 6 | 0.49 |
| (2,1291) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 5 | 0.49 |
| (2,1291) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 19 | 0.49 |
| (2,1288) | 1:167:A:LEU:HD23 | 1:167:A:LEU:HA | 2 | 0.49 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 14 | 0.49 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 16 | 0.49 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 10 | 0.49 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 13 | 0.49 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 19 | 0.49 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 20 | 0.49 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB2 | 4 | 0.49 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 4 | 0.49 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 9 | 0.49 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 13 | 0.49 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 19 | 0.49 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 8 | 0.49 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 15 | 0.49 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 14 | 0.49 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 5 | 0.49 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 8 | 0.49 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 11 | 0.49 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 14 | 0.49 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 16 | 0.49 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 1 | 0.48 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 3 | 0.48 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 14 | 0.48 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 17 | 0.48 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 7 | 0.48 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 1 | 0.48 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 12 | 0.48 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 15 | 0.48 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 2 | 0.48 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 4 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 12 | 0.48 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 15 | 0.48 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 11 | 0.48 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 14 | 0.48 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 15 | 0.48 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 17 | 0.48 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 4 | 0.48 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 9 | 0.48 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 5 | 0.48 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 14 | 0.48 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 9 | 0.48 |
| (4,278) | 1:142:A:VAL:HG12 | 1:102:A:ALA:H | 12 | 0.48 |
| (4,204) | 1:173:A:ALA:HB1 | 1:111:A:LYS:HG3 | 5 | 0.48 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 9 | 0.48 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 3 | 0.48 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 17 | 0.48 |
| (4,95) | 1:51:A:GLU:H | 1:58:A:GLU:HG3 | 18 | 0.48 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 15 | 0.48 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 8 | 0.48 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 12 | 0.48 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 11 | 0.48 |
| (2,3964) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H6N | 20 | 0.48 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 10 | 0.48 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 7 | 0.48 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 9 | 0.48 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 17 | 0.48 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 6 | 0.48 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 20 | 0.48 |
| (2,3832) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 11 | 0.48 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 11 | 0.48 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 13 | 0.48 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 9 | 0.48 |
| (2,3798) | 1:48:A:ILE:HD11 | 1:48:A:ILE:HG13 | 18 | 0.48 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 20 | 0.48 |
| (2,3676) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 6 | 0.48 |
| (2,3676) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 8 | 0.48 |
| (2,3676) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 12 | 0.48 |
| (2,3676) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 16 | 0.48 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 6 | 0.48 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 5 | 0.48 |
| (2,3514) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 17 | 0.48 |
| (2,3415) | 1:122:A:VAL:HG22 | 1:122:A:VAL:H | 19 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 18 | 0.48 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 5 | 0.48 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 15 | 0.48 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 3 | 0.48 |
| (2,2521) | 1:105:A:ASN:H | 1:102:A:ALA:HB3 | 8 | 0.48 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 4 | 0.48 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 9 | 0.48 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 1 | 0.48 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 3 | 0.48 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 4 | 0.48 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 20 | 0.48 |
| (2,1859) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 18 | 0.48 |
| (2,1851) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 8 | 0.48 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 10 | 0.48 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 18 | 0.48 |
| (2,1823) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE3 | 19 | 0.48 |
| (2,1821) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 6 | 0.48 |
| (2,1821) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 7 | 0.48 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 10 | 0.48 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 12 | 0.48 |
| (2,1744) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 19 | 0.48 |
| (2,1744) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 20 | 0.48 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 1 | 0.48 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 3 | 0.48 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 4 | 0.48 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 7 | 0.48 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 11 | 0.48 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 14 | 0.48 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 15 | 0.48 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 19 | 0.48 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 3 | 0.48 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 15 | 0.48 |
| (2,1531) | 1:21:A:LEU:HD11 | 1:14:A:VAL:HA | 1 | 0.48 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 4 | 0.48 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 6 | 0.48 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 9 | 0.48 |
| (2,1435) | 1:15:A:LEU:HD23 | 1:15:A:LEU:H | 5 | 0.48 |
| (2,1435) | 1:15:A:LEU:HD22 | 1:15:A:LEU:H | 20 | 0.48 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 5 | 0.48 |
| (2,1407) | 1:95:A:ALA:HB3 | 1:95:A:ALA:H | 19 | 0.48 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 16 | 0.48 |
| (2,1377) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 12 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 18 | 0.48 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 7 | 0.48 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 12 | 0.48 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 18 | 0.48 |
| (2,1281) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HD1 | 2 | 0.48 |
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 16 | 0.48 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 5 | 0.48 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 7 | 0.48 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 9 | 0.48 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 13 | 0.48 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 18 | 0.48 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 4 | 0.48 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 14 | 0.48 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 6 | 0.48 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 13 | 0.48 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 13 | 0.48 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 6 | 0.48 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 14 | 0.48 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 10 | 0.48 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 12 | 0.48 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 2 | 0.48 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 11 | 0.48 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 15 | 0.48 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 20 | 0.48 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 2 | 0.48 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 14 | 0.48 |
| (2,203) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 12 | 0.48 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 17 | 0.48 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 1 | 0.48 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 4 | 0.48 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 7 | 0.48 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 12 | 0.48 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 17 | 0.48 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 18 | 0.48 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 20 | 0.48 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 8 | 0.47 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 15 | 0.47 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 10 | 0.47 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 20 | 0.47 |
| (4,446) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HG | 5 | 0.47 |
| (4,446) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HG | 16 | 0.47 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 14 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 17 | 0.47 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 9 | 0.47 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 20 | 0.47 |
| (4,415) | 1:19:A:PRO:HB3 | 1:36:A:GLU:HG2 | 1 | 0.47 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 20 | 0.47 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 18 | 0.47 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 19 | 0.47 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 1 | 0.47 |
| (4,311) | 1:143:A:VAL:HG12 | 1:178:A:VAL:HA | 9 | 0.47 |
| (4,303) | 1:110:A:LEU:HD13 | 1:107:A:ASP:HA | 5 | 0.47 |
| (4,301) | 1:97:A:LEU:HD22 | 1:156:A:PHE:HB2 | 5 | 0.47 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 2 | 0.47 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 20 | 0.47 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB2 | 7 | 0.47 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 2 | 0.47 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 2 | 0.47 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 6 | 0.47 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 10 | 0.47 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 15 | 0.47 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 2 | 0.47 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 5 | 0.47 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 12 | 0.47 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 4 | 0.47 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 12 | 0.47 |
| (2,3832) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 7 | 0.47 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD21 | 3 | 0.47 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 19 | 0.47 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 19 | 0.47 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 18 | 0.47 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 3 | 0.47 |
| (2,3782) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 6 | 0.47 |
| (2,3782) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 7 | 0.47 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 5 | 0.47 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 16 | 0.47 |
| (2,3749) | 1:44:A:LYS:HG3 | 1:21:A:LEU:HD22 | 20 | 0.47 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 19 | 0.47 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 13 | 0.47 |
| (2,3676) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 14 | 0.47 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 13 | 0.47 |
| (2,3527) | 1:84:A:VAL:HG23 | 1:85:A:ASP:HB2 | 5 | 0.47 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 10 | 0.47 |
| (2,3492) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 5 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3466) | 1:97:A:LEU:HD21 | 1:166:A:TRP:HB2 | 2 | 0.47 |
| (2,3459) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 2 | 0.47 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 13 | 0.47 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 17 | 0.47 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 4 | 0.47 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 12 | 0.47 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 16 | 0.47 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 18 | 0.47 |
| (2,3391) | 1:56:A:ILE:HG23 | 1:65:A:PHE:HD1 | 9 | 0.47 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 7 | 0.47 |
| (2,3355) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 5 | 0.47 |
| (2,3346) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 12 | 0.47 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 8 | 0.47 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 7 | 0.47 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 10 | 0.47 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 17 | 0.47 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 1 | 0.47 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 2 | 0.47 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 3 | 0.47 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 8 | 0.47 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 11 | 0.47 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 19 | 0.47 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG22 | 5 | 0.47 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 6 | 0.47 |
| (2,1859) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 9 | 0.47 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 14 | 0.47 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 15 | 0.47 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 17 | 0.47 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 15 | 0.47 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 17 | 0.47 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 18 | 0.47 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 14 | 0.47 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 19 | 0.47 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 17 | 0.47 |
| (2,1823) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE3 | 13 | 0.47 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 1 | 0.47 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 2 | 0.47 |
| (2,1821) | 1:143:A:VAL:HG21 | 1:143:A:VAL:HB | 5 | 0.47 |
| (2,1821) | 1:143:A:VAL:HG21 | 1:143:A:VAL:HB | 16 | 0.47 |
| (2,1821) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 19 | 0.47 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 8 | 0.47 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 9 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 10 | 0.47 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 6 | 0.47 |
| (2,1813) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HG | 6 | 0.47 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 4 | 0.47 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 1 | 0.47 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 3 | 0.47 |
| (2,1744) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 9 | 0.47 |
| (2,1744) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 15 | 0.47 |
| (2,1710) | 1:26:A:LEU:HD22 | 1:15:A:LEU:HA | 19 | 0.47 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 14 | 0.47 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 1 | 0.47 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 12 | 0.47 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 13 | 0.47 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 16 | 0.47 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 18 | 0.47 |
| (2,1490) | 1:167:A:LEU:HD12 | 1:166:A:TRP:HA | 9 | 0.47 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 11 | 0.47 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 5 | 0.47 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 3 | 0.47 |
| (2,1424) | 1:56:A:ILE:HG21 | 1:65:A:PHE:HE1 | 14 | 0.47 |
| (2,1388) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 17 | 0.47 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 19 | 0.47 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 8 | 0.47 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 5 | 0.47 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 15 | 0.47 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 19 | 0.47 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 16 | 0.47 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 8 | 0.47 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 18 | 0.47 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 6 | 0.47 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 7 | 0.47 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 6 | 0.47 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 5 | 0.47 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 16 | 0.47 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 16 | 0.47 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 18 | 0.47 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 10 | 0.47 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 20 | 0.47 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 20 | 0.47 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 16 | 0.47 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 5 | 0.47 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 18 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 9 | 0.47 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 12 | 0.47 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 2 | 0.47 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 6 | 0.47 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 13 | 0.47 |
| (2,16) | 1:21:A:LEU:HD13 | 1:10:A:PHE:HE1 | 20 | 0.47 |
| (4,449) | 1:74:A:ILE:HD13 | 1:57:A:VAL:HG23 | 12 | 0.46 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 3 | 0.46 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 4 | 0.46 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 11 | 0.46 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 12 | 0.46 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 16 | 0.46 |
| (4,446) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HG | 11 | 0.46 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 3 | 0.46 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 9 | 0.46 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 10 | 0.46 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 3 | 0.46 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 6 | 0.46 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 10 | 0.46 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 2 | 0.46 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 5 | 0.46 |
| (4,204) | 1:173:A:ALA:HB2 | 1:114:A:ILE:HG13 | 12 | 0.46 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 10 | 0.46 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 8 | 0.46 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 11 | 0.46 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 4 | 0.46 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 10 | 0.46 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 14 | 0.46 |
| (2,3843) | 1:76:A:ALA:HB1 | 1:16:A:ARG:HA | 5 | 0.46 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 19 | 0.46 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 6 | 0.46 |
| (2,3832) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 16 | 0.46 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 7 | 0.46 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 20 | 0.46 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 8 | 0.46 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 13 | 0.46 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 1 | 0.46 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 2 | 0.46 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 3 | 0.46 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 12 | 0.46 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 9 | 0.46 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 12 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 1 | 0.46 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 2 | 0.46 |
| (2,3782) | 1:143:A:VAL:HG21 | 1:143:A:VAL:HB | 16 | 0.46 |
| (2,3782) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 19 | 0.46 |
| (2,3761) | 1:117:A:MET:HE1 | 1:117:A:MET:HB2 | 20 | 0.46 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 4 | 0.46 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 13 | 0.46 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 6 | 0.46 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 15 | 0.46 |
| (2,3570) | 1:4:A:MET:HE2 | 1:52:A:GLU:HA | 11 | 0.46 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 17 | 0.46 |
| (2,3514) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 14 | 0.46 |
| (2,3490) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HA | 18 | 0.46 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 8 | 0.46 |
| (2,3467) | 1:11:A:LEU:HD12 | 1:38:A:LEU:HA | 6 | 0.46 |
| (2,3434) | 1:15:A:LEU:HD12 | 1:65:A:PHE:HE1 | 20 | 0.46 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 8 | 0.46 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 19 | 0.46 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 9 | 0.46 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 11 | 0.46 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 18 | 0.46 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 3 | 0.46 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 20 | 0.46 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 18 | 0.46 |
| (2,3177) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 4 | 0.46 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 3 | 0.46 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 11 | 0.46 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 13 | 0.46 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 17 | 0.46 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 7 | 0.46 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 9 | 0.46 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 11 | 0.46 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 18 | 0.46 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 19 | 0.46 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 17 | 0.46 |
| (2,1877) | 1:129:A:THR:HG21 | 1:129:A:THR:HA | 20 | 0.46 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 9 | 0.46 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 3 | 0.46 |
| (2,1859) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 2 | 0.46 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 2 | 0.46 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 6 | 0.46 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 19 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1827) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HG | 2 | 0.46 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 5 | 0.46 |
| (2,1827) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HG | 9 | 0.46 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 3 | 0.46 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 8 | 0.46 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 10 | 0.46 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 12 | 0.46 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 20 | 0.46 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 15 | 0.46 |
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 1 | 0.46 |
| (2,1819) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HG | 5 | 0.46 |
| (2,1819) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HG | 6 | 0.46 |
| (2,1819) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HG | 7 | 0.46 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 19 | 0.46 |
| (2,1793) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HB2 | 10 | 0.46 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 11 | 0.46 |
| (2,1744) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 8 | 0.46 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 14 | 0.46 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 20 | 0.46 |
| (2,1568) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 5 | 0.46 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 5 | 0.46 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 3 | 0.46 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 7 | 0.46 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 11 | 0.46 |
| (2,1490) | 1:167:A:LEU:HD13 | 1:166:A:TRP:HA | 19 | 0.46 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 11 | 0.46 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 20 | 0.46 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 9 | 0.46 |
| (2,1377) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 18 | 0.46 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 17 | 0.46 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 7 | 0.46 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 9 | 0.46 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 2 | 0.46 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 3 | 0.46 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 13 | 0.46 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 14 | 0.46 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 16 | 0.46 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 19 | 0.46 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 6 | 0.46 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 8 | 0.46 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 17 | 0.46 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 9 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 6 | 0.46 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 17 | 0.46 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 3 | 0.46 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 2 | 0.46 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 2 | 0.46 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 10 | 0.46 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 1 | 0.46 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 17 | 0.46 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 1 | 0.46 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 6 | 0.46 |
| (2,405) | 1:95:A:ALA:HB2 | 1:149:A:LYS:H | 7 | 0.46 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 6 | 0.46 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 4 | 0.46 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 5 | 0.46 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 19 | 0.46 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 1 | 0.46 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 10 | 0.46 |
| (2,32) | 1:88:A:TYR:HE1 | 1:159:A:TYR:HD1 | 2 | 0.46 |
| (2,19) | 1:13:A:LEU:HA | 1:17:A:HIS:HD2 | 16 | 0.46 |
| (4,450) | 1:97:A:LEU:HD22 | 1:124:A:LEU:HD23 | 16 | 0.45 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 7 | 0.45 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 9 | 0.45 |
| (4,446) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HG | 10 | 0.45 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 20 | 0.45 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD11 | 7 | 0.45 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 17 | 0.45 |
| (4,320) | 1:151:A:MET:HE1 | 1:147:A:ASP:HB2 | 3 | 0.45 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 13 | 0.45 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 1 | 0.45 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 3 | 0.45 |
| (4,274) | 1:124:A:LEU:HD21 | 1:156:A:PHE:HZ | 9 | 0.45 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 18 | 0.45 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 4 | 0.45 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 4 | 0.45 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD11 | 15 | 0.45 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 2 | 0.45 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 10 | 0.45 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 17 | 0.45 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 10 | 0.45 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 16 | 0.45 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 4 | 0.45 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD21 | 16 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3821) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 8 | 0.45 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 15 | 0.45 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 19 | 0.45 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 3 | 0.45 |
| (2,3782) | 1:143:A:VAL:HG21 | 1:143:A:VAL:HB | 5 | 0.45 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 8 | 0.45 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 10 | 0.45 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 20 | 0.45 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 14 | 0.45 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 1 | 0.45 |
| (2,3676) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 4 | 0.45 |
| (2,3676) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 7 | 0.45 |
| (2,3570) | 1:4:A:MET:HE3 | 1:52:A:GLU:HA | 16 | 0.45 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 12 | 0.45 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 3 | 0.45 |
| (2,3514) | 1:143:A:VAL:HG12 | 1:132:A:ARG:HA | 15 | 0.45 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 14 | 0.45 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 7 | 0.45 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 20 | 0.45 |
| (2,3428) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 7 | 0.45 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 2 | 0.45 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 3 | 0.45 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 5 | 0.45 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 7 | 0.45 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 11 | 0.45 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 12 | 0.45 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 7 | 0.45 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 2 | 0.45 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 6 | 0.45 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 13 | 0.45 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 6 | 0.45 |
| (2,3344) | 1:41:A:MET:HE2 | 1:10:A:PHE:HD1 | 5 | 0.45 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 1 | 0.45 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 11 | 0.45 |
| (2,3079) | 1:118:A:SER:H | 2:201:A:NAD:H51A | 1 | 0.45 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 4 | 0.45 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 5 | 0.45 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 10 | 0.45 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 4 | 0.45 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 10 | 0.45 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 13 | 0.45 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 18 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 17 | 0.45 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 3 | 0.45 |
| (2,1859) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 4 | 0.45 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 6 | 0.45 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 14 | 0.45 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 9 | 0.45 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 16 | 0.45 |
| (2,1827) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HG | 8 | 0.45 |
| (2,1827) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HG | 17 | 0.45 |
| (2,1823) | 1:37:A:LEU:HD13 | 1:41:A:MET:HE1 | 9 | 0.45 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 4 | 0.45 |
| (2,1821) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 9 | 0.45 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 11 | 0.45 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 15 | 0.45 |
| (2,1821) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 17 | 0.45 |
| (2,1821) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 18 | 0.45 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 18 | 0.45 |
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 11 | 0.45 |
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 17 | 0.45 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 6 | 0.45 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 12 | 0.45 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 17 | 0.45 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 3 | 0.45 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 16 | 0.45 |
| (2,1601) | 1:41:A:MET:HE2 | 1:10:A:PHE:HB3 | 7 | 0.45 |
| (2,1588) | 1:152:A:ALA:HB2 | 1:149:A:LYS:HA | 14 | 0.45 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 9 | 0.45 |
| (2,1554) | 1:38:A:LEU:HD21 | 1:50:A:MET:HG2 | 16 | 0.45 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 17 | 0.45 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 15 | 0.45 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 4 | 0.45 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 15 | 0.45 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 1 | 0.45 |
| (2,1314) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 14 | 0.45 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 19 | 0.45 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 1 | 0.45 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 4 | 0.45 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 18 | 0.45 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 20 | 0.45 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 4 | 0.45 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 8 | 0.45 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 11 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 15 | 0.45 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 20 | 0.45 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 15 | 0.45 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 2 | 0.45 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 4 | 0.45 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 8 | 0.45 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 6 | 0.45 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 4 | 0.45 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 3 | 0.45 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 1 | 0.45 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 14 | 0.45 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 18 | 0.45 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 3 | 0.45 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 4 | 0.45 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 12 | 0.45 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 20 | 0.45 |
| (2,30) | 1:88:A:TYR:HD1 | 1:159:A:TYR:HE1 | 13 | 0.45 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 11 | 0.45 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 2 | 0.44 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 19 | 0.44 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 4 | 0.44 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 11 | 0.44 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 17 | 0.44 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 19 | 0.44 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 8 | 0.44 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 19 | 0.44 |
| (4,368) | 1:20:A:ALA:HB1 | 1:22:A:ILE:HB | 10 | 0.44 |
| (4,328) | 1:122:A:VAL:HG12 | 1:113:A:GLY:HA2 | 14 | 0.44 |
| (4,320) | 1:151:A:MET:HE3 | 1:158:A:PHE:HB3 | 11 | 0.44 |
| (4,129) | 1:13:A:LEU:HD23 | 1:18:A:ASN:H | 12 | 0.44 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD21 | 8 | 0.44 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 15 | 0.44 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 9 | 0.44 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 13 | 0.44 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 18 | 0.44 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 1 | 0.44 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 7 | 0.44 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD23 | 20 | 0.44 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 4 | 0.44 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 8 | 0.44 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 15 | 0.44 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 9 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 7 | 0.44 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 6 | 0.44 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 17 | 0.44 |
| (2,3791) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 7 | 0.44 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 4 | 0.44 |
| (2,3782) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 9 | 0.44 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 11 | 0.44 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 12 | 0.44 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 15 | 0.44 |
| (2,3782) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 18 | 0.44 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 18 | 0.44 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 9 | 0.44 |
| (2,3676) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 19 | 0.44 |
| (2,3600) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 8 | 0.44 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 4 | 0.44 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 2 | 0.44 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 1 | 0.44 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 18 | 0.44 |
| (2,3427) | 1:165:A:VAL:HG13 | 2:201:A:NAD:H5N | 7 | 0.44 |
| (2,3415) | 1:122:A:VAL:HG21 | 1:122:A:VAL:H | 11 | 0.44 |
| (2,3415) | 1:122:A:VAL:HG22 | 1:122:A:VAL:H | 18 | 0.44 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 4 | 0.44 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 10 | 0.44 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 16 | 0.44 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 19 | 0.44 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 7 | 0.44 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 8 | 0.44 |
| (2,3399) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 14 | 0.44 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 17 | 0.44 |
| (2,3346) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 18 | 0.44 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 16 | 0.44 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 19 | 0.44 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 10 | 0.44 |
| (2,2748) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 13 | 0.44 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 8 | 0.44 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 16 | 0.44 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 6 | 0.44 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 8 | 0.44 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 13 | 0.44 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 2 | 0.44 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 6 | 0.44 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 11 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 15 | 0.44 |
| (2,1877) | 1:129:A:THR:HG22 | 1:129:A:THR:HA | 2 | 0.44 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 13 | 0.44 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 1 | 0.44 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 11 | 0.44 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG22 | 10 | 0.44 |
| (2,1856) | 1:22:A:ILE:HD11 | 1:14:A:VAL:HG21 | 13 | 0.44 |
| (2,1851) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD13 | 5 | 0.44 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 7 | 0.44 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 7 | 0.44 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 8 | 0.44 |
| (2,1827) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HG | 7 | 0.44 |
| (2,1827) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HG | 13 | 0.44 |
| (2,1821) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 14 | 0.44 |
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 3 | 0.44 |
| (2,1819) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HG | 4 | 0.44 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 18 | 0.44 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 15 | 0.44 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 15 | 0.44 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 19 | 0.44 |
| (2,1744) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HA | 11 | 0.44 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 16 | 0.44 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 18 | 0.44 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG21 | 4 | 0.44 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 10 | 0.44 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 11 | 0.44 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 8 | 0.44 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 14 | 0.44 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 7 | 0.44 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 17 | 0.44 |
| (2,1426) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HD1 | 13 | 0.44 |
| (2,1407) | 1:95:A:ALA:HB3 | 1:95:A:ALA:H | 7 | 0.44 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 8 | 0.44 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 11 | 0.44 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 15 | 0.44 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 16 | 0.44 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 17 | 0.44 |
| (2,1211) | 1:177:A:LYS:HD2 | 1:177:A:LYS:HA | 11 | 0.44 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 6 | 0.44 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 10 | 0.44 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 8 | 0.44 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 12 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 19 | 0.44 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 20 | 0.44 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 1 | 0.44 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 19 | 0.44 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 16 | 0.44 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 1 | 0.44 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 4 | 0.44 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 8 | 0.44 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 18 | 0.44 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 4 | 0.44 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB1 | 2 | 0.44 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 20 | 0.44 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 7 | 0.44 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 13 | 0.44 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 13 | 0.44 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 3 | 0.44 |
| (2,339) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 6 | 0.44 |
| (2,300) | 1:153:A:ASP:H | 1:95:A:ALA:HB1 | 6 | 0.44 |
| (2,233) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 1 | 0.44 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 6 | 0.44 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 8 | 0.44 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 9 | 0.44 |
| (2,175) | 1:53:A:LEU:HD22 | 1:56:A:ILE:H | 6 | 0.44 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 7 | 0.44 |
| (2,175) | 1:53:A:LEU:HD22 | 1:56:A:ILE:H | 16 | 0.44 |
| (2,19) | 1:13:A:LEU:HA | 1:17:A:HIS:HD2 | 20 | 0.44 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 13 | 0.44 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HG3 | 20 | 0.43 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 6 | 0.43 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 13 | 0.43 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD11 | 15 | 0.43 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 8 | 0.43 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 18 | 0.43 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 19 | 0.43 |
| (4,413) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 19 | 0.43 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 20 | 0.43 |
| (4,316) | 1:37:A:LEU:HD22 | 1:8:A:SER:HB2 | 2 | 0.43 |
| (4,311) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 10 | 0.43 |
| (4,300) | 1:97:A:LEU:HD23 | 1:156:A:PHE:HB3 | 11 | 0.43 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 18 | 0.43 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 1 | 0.43 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 6 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,259) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 20 | 0.43 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 1 | 0.43 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD2 | 8 | 0.43 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB2 | 4 | 0.43 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 10 | 0.43 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 2 | 0.43 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 7 | 0.43 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 20 | 0.43 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 11 | 0.43 |
| (2,3836) | 1:168:A:ILE:HD12 | 1:171:A:VAL:HG13 | 5 | 0.43 |
| (2,3833) | 1:168:A:ILE:HD11 | 1:168:A:ILE:HG13 | 12 | 0.43 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 20 | 0.43 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 20 | 0.43 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 8 | 0.43 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 10 | 0.43 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 1 | 0.43 |
| (2,3782) | 1:143:A:VAL:HG23 | 1:143:A:VAL:HB | 14 | 0.43 |
| (2,3782) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 17 | 0.43 |
| (2,3781) | 1:142:A:VAL:HG11 | 1:142:A:VAL:HB | 2 | 0.43 |
| (2,3742) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG2 | 13 | 0.43 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 15 | 0.43 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG23 | 17 | 0.43 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 19 | 0.43 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 2 | 0.43 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 3 | 0.43 |
| (2,3676) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 5 | 0.43 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 10 | 0.43 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 11 | 0.43 |
| (2,3676) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 17 | 0.43 |
| (2,3607) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 19 | 0.43 |
| (2,3600) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 2 | 0.43 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE1 | 9 | 0.43 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE2 | 2 | 0.43 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 9 | 0.43 |
| (2,3544) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 10 | 0.43 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 13 | 0.43 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 17 | 0.43 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 19 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 2 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 6 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 8 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 9 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 10 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 12 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 16 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 17 | 0.43 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 18 | 0.43 |
| (2,3527) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 18 | 0.43 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 6 | 0.43 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 12 | 0.43 |
| (2,3466) | 1:97:A:LEU:HD22 | 1:166:A:TRP:HB2 | 20 | 0.43 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 1 | 0.43 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 7 | 0.43 |
| (2,3439) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 13 | 0.43 |
| (2,3430) | 1:128:A:ILE:HD13 | 1:127:A:ASP:H | 14 | 0.43 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 1 | 0.43 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 6 | 0.43 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 8 | 0.43 |
| (2,3411) | 1:56:A:ILE:HG23 | 1:56:A:ILE:H | 9 | 0.43 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 20 | 0.43 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 1 | 0.43 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 8 | 0.43 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 9 | 0.43 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 13 | 0.43 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 2 | 0.43 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 10 | 0.43 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 11 | 0.43 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 15 | 0.43 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 17 | 0.43 |
| (2,3177) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 2 | 0.43 |
| (2,3177) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 3 | 0.43 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD21 | 7 | 0.43 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 13 | 0.43 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 17 | 0.43 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 19 | 0.43 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 1 | 0.43 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 8 | 0.43 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 15 | 0.43 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 10 | 0.43 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 14 | 0.43 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 15 | 0.43 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 7 | 0.43 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 8 | 0.43 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 15 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 1 | 0.43 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 16 | 0.43 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 5 | 0.43 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 19 | 0.43 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 4 | 0.43 |
| (2,1834) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 11 | 0.43 |
| (2,1825) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 16 | 0.43 |
| (2,1821) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 13 | 0.43 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 20 | 0.43 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 11 | 0.43 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 12 | 0.43 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 8 | 0.43 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 14 | 0.43 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 20 | 0.43 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 5 | 0.43 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 2 | 0.43 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 8 | 0.43 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 12 | 0.43 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 2 | 0.43 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 4 | 0.43 |
| (2,1744) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HA | 5 | 0.43 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 6 | 0.43 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 7 | 0.43 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 17 | 0.43 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 6 | 0.43 |
| (2,1588) | 1:152:A:ALA:HB2 | 1:149:A:LYS:HA | 2 | 0.43 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 2 | 0.43 |
| (2,1541) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 12 | 0.43 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 16 | 0.43 |
| (2,1534) | 1:151:A:MET:HE2 | 1:151:A:MET:HA | 4 | 0.43 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 19 | 0.43 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 16 | 0.43 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 10 | 0.43 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 12 | 0.43 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 1 | 0.43 |
| (2,1435) | 1:15:A:LEU:HD22 | 1:15:A:LEU:H | 4 | 0.43 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 3 | 0.43 |
| (2,1388) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 16 | 0.43 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 15 | 0.43 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 2 | 0.43 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 3 | 0.43 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 5 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 14 | 0.43 |
| (2,1295) | 1:57:A:VAL:HG11 | 1:57:A:VAL:HA | 1 | 0.43 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 11 | 0.43 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 3 | 0.43 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 8 | 0.43 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 9 | 0.43 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 11 | 0.43 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 16 | 0.43 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 2 | 0.43 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 18 | 0.43 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 5 | 0.43 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 6 | 0.43 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 9 | 0.43 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 12 | 0.43 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 15 | 0.43 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 17 | 0.43 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 6 | 0.43 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 9 | 0.43 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 17 | 0.43 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 5 | 0.43 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 19 | 0.43 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 17 | 0.43 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 1 | 0.43 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 8 | 0.43 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 14 | 0.43 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD22 | 3 | 0.43 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 15 | 0.43 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 15 | 0.43 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD23 | 20 | 0.43 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 16 | 0.43 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 9 | 0.43 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 9 | 0.43 |
| (2,29) | 1:88:A:TYR:HD1 | 1:159:A:TYR:HD1 | 12 | 0.43 |
| (2,19) | 1:13:A:LEU:HA | 1:17:A:HIS:HD2 | 7 | 0.43 |
| (2,16) | 1:21:A:LEU:HD13 | 1:10:A:PHE:HE1 | 8 | 0.43 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 8 | 0.42 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 1 | 0.42 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 2 | 0.42 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 2 | 0.42 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 5 | 0.42 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 8 | 0.42 |
| (4,437) | 1:178:A:VAL:HG21 | 1:177:A:LYS:HG2 | 9 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 13 | 0.42 |
| (4,413) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 16 | 0.42 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 8 | 0.42 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 15 | 0.42 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 11 | 0.42 |
| (4,311) | 1:143:A:VAL:HG12 | 1:178:A:VAL:HA | 14 | 0.42 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 15 | 0.42 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 17 | 0.42 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 3 | 0.42 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 5 | 0.42 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 6 | 0.42 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 12 | 0.42 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 14 | 0.42 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 16 | 0.42 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 19 | 0.42 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 13 | 0.42 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD22 | 3 | 0.42 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 3 | 0.42 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 1 | 0.42 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 12 | 0.42 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 8 | 0.42 |
| (2,3811) | 1:15:A:LEU:HD11 | 1:74:A:ILE:HD12 | 17 | 0.42 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 5 | 0.42 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 9 | 0.42 |
| (2,3798) | 1:48:A:ILE:HD12 | 1:48:A:ILE:HG13 | 13 | 0.42 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 14 | 0.42 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 16 | 0.42 |
| (2,3797) | 1:146:A:VAL:HG11 | 1:174:A:GLU:HG2 | 5 | 0.42 |
| (2,3782) | 1:143:A:VAL:HG22 | 1:143:A:VAL:HB | 13 | 0.42 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 7 | 0.42 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 7 | 0.42 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 6 | 0.42 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 13 | 0.42 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 1 | 0.42 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 4 | 0.42 |
| (2,3544) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 7 | 0.42 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 16 | 0.42 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 4 | 0.42 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 13 | 0.42 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 14 | 0.42 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 15 | 0.42 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 19 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 20 | 0.42 |
| (2,3514) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 10 | 0.42 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 13 | 0.42 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 5 | 0.42 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 4 | 0.42 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 16 | 0.42 |
| (2,3411) | 1:56:A:ILE:HG21 | 1:56:A:ILE:H | 14 | 0.42 |
| (2,3411) | 1:56:A:ILE:HG22 | 1:56:A:ILE:H | 15 | 0.42 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 3 | 0.42 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 9 | 0.42 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 18 | 0.42 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 19 | 0.42 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 14 | 0.42 |
| (2,3265) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 7 | 0.42 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 1 | 0.42 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 6 | 0.42 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD21 | 1 | 0.42 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD21 | 16 | 0.42 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 16 | 0.42 |
| (2,2738) | 1:30:A:GLY:H | 1:26:A:LEU:HD21 | 3 | 0.42 |
| (2,2521) | 1:105:A:ASN:H | 1:102:A:ALA:HB3 | 15 | 0.42 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 12 | 0.42 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 17 | 0.42 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 2 | 0.42 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 4 | 0.42 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 2 | 0.42 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 5 | 0.42 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 9 | 0.42 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 14 | 0.42 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 16 | 0.42 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 19 | 0.42 |
| (2,1872) | 1:168:A:ILE:HD11 | 1:168:A:ILE:HG13 | 5 | 0.42 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 14 | 0.42 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 18 | 0.42 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 15 | 0.42 |
| (2,1834) | 1:14:A:VAL:HG22 | 1:21:A:LEU:HG | 13 | 0.42 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 13 | 0.42 |
| (2,1819) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HG | 8 | 0.42 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 3 | 0.42 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 9 | 0.42 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 12 | 0.42 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 13 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 13 | 0.42 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 15 | 0.42 |
| (2,1500) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 20 | 0.42 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 2 | 0.42 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 2 | 0.42 |
| (2,1377) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 7 | 0.42 |
| (2,1377) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 9 | 0.42 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 6 | 0.42 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 13 | 0.42 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 10 | 0.42 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 15 | 0.42 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 6 | 0.42 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 16 | 0.42 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 9 | 0.42 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 2 | 0.42 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 2 | 0.42 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 7 | 0.42 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 13 | 0.42 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 9 | 0.42 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 12 | 0.42 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 19 | 0.42 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 20 | 0.42 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 14 | 0.42 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 8 | 0.42 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 10 | 0.42 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 16 | 0.42 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 17 | 0.42 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 8 | 0.42 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 11 | 0.42 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 19 | 0.42 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 4 | 0.42 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 12 | 0.42 |
| (2,118) | 1:171:A:VAL:H | 1:171:A:VAL:HG21 | 15 | 0.42 |
| (2,16) | 1:21:A:LEU:HD13 | 1:10:A:PHE:HE1 | 1 | 0.42 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 2 | 0.42 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 13 | 0.41 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 17 | 0.41 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 6 | 0.41 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG22 | 16 | 0.41 |
| (4,325) | 1:7:A:VAL:HG13 | 1:10:A:PHE:HB3 | 16 | 0.41 |
| (4,320) | 1:151:A:MET:HE3 | 1:158:A:PHE:HB3 | 2 | 0.41 |
| (4,195) | 1:114:A:ILE:HD11 | 1:117:A:MET:HE1 | 6 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 4 | 0.41 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 5 | 0.41 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 16 | 0.41 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD12 | 20 | 0.41 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 18 | 0.41 |
| (2,3899) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 2 | 0.41 |
| (2,3834) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 15 | 0.41 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 1 | 0.41 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 2 | 0.41 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 8 | 0.41 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 11 | 0.41 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 19 | 0.41 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 8 | 0.41 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 12 | 0.41 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 20 | 0.41 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 7 | 0.41 |
| (2,3798) | 1:48:A:ILE:HD11 | 1:48:A:ILE:HG13 | 11 | 0.41 |
| (2,3798) | 1:48:A:ILE:HD11 | 1:48:A:ILE:HG13 | 20 | 0.41 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 1 | 0.41 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 5 | 0.41 |
| (2,3761) | 1:117:A:MET:HE1 | 1:117:A:MET:HB2 | 17 | 0.41 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 5 | 0.41 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 11 | 0.41 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 17 | 0.41 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 13 | 0.41 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 2 | 0.41 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 11 | 0.41 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 19 | 0.41 |
| (2,3666) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 18 | 0.41 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 3 | 0.41 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 8 | 0.41 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 11 | 0.41 |
| (2,3544) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 18 | 0.41 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 1 | 0.41 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 3 | 0.41 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 7 | 0.41 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 11 | 0.41 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 5 | 0.41 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 10 | 0.41 |
| (2,3482) | 1:38:A:LEU:HD22 | 1:49:A:SER:HA | 8 | 0.41 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 4 | 0.41 |
| (2,3439) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 11 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3428) | 1:108:A:LEU:HD12 | 2:201:A:NAD:H2A | 5 | 0.41 |
| (2,3415) | 1:122:A:VAL:HG23 | 1:122:A:VAL:H | 12 | 0.41 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 4 | 0.41 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 12 | 0.41 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 13 | 0.41 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 13 | 0.41 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 15 | 0.41 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 3 | 0.41 |
| (2,3346) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 7 | 0.41 |
| (2,3346) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 9 | 0.41 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 17 | 0.41 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 19 | 0.41 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 20 | 0.41 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 17 | 0.41 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 7 | 0.41 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 7 | 0.41 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 10 | 0.41 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 2 | 0.41 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 3 | 0.41 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 12 | 0.41 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 17 | 0.41 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 15 | 0.41 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 8 | 0.41 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 11 | 0.41 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 17 | 0.41 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 11 | 0.41 |
| (2,1834) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 12 | 0.41 |
| (2,1827) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HG | 6 | 0.41 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 7 | 0.41 |
| (2,1819) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HG | 12 | 0.41 |
| (2,1819) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HG | 18 | 0.41 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 11 | 0.41 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 17 | 0.41 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 9 | 0.41 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 20 | 0.41 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 5 | 0.41 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 20 | 0.41 |
| (2,1744) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HA | 1 | 0.41 |
| (2,1744) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 13 | 0.41 |
| (2,1744) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 17 | 0.41 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 2 | 0.41 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 9 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 11 | 0.41 |
| (2,1699) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 18 | 0.41 |
| (2,1599) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 10 | 0.41 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 13 | 0.41 |
| (2,1555) | 1:84:A:VAL:HG21 | 1:85:A:ASP:HB2 | 15 | 0.41 |
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 3 | 0.41 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 18 | 0.41 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 15 | 0.41 |
| (2,1377) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 16 | 0.41 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 2 | 0.41 |
| (2,1314) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 8 | 0.41 |
| (2,1311) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 17 | 0.41 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 12 | 0.41 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 14 | 0.41 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 7 | 0.41 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 7 | 0.41 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 15 | 0.41 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 1 | 0.41 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 5 | 0.41 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 13 | 0.41 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 16 | 0.41 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 18 | 0.41 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 19 | 0.41 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 4 | 0.41 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 20 | 0.41 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 12 | 0.41 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 17 | 0.41 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 4 | 0.41 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 12 | 0.41 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 3 | 0.41 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 6 | 0.41 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 2 | 0.41 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 12 | 0.41 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD23 | 13 | 0.41 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 2 | 0.41 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 15 | 0.41 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 8 | 0.41 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 1 | 0.41 |
| (2,29) | 1:88:A:TYR:HD1 | 1:159:A:TYR:HD1 | 14 | 0.41 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 20 | 0.4 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 13 | 0.4 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 10 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 3 | 0.4 |
| (4,332) | 1:37:A:LEU:HD12 | 1:41:A:MET:HB2 | 20 | 0.4 |
| (4,259) | 1:117:A:MET:HE3 | 2:201:A:NAD:H2A | 10 | 0.4 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 15 | 0.4 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 19 | 0.4 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 19 | 0.4 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 17 | 0.4 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD23 | 16 | 0.4 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 9 | 0.4 |
| (2,3824) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 5 | 0.4 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 14 | 0.4 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 2 | 0.4 |
| (2,3811) | 1:15:A:LEU:HD13 | 1:74:A:ILE:HD11 | 12 | 0.4 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 3 | 0.4 |
| (2,3791) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 6 | 0.4 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 16 | 0.4 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 19 | 0.4 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 11 | 0.4 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 13 | 0.4 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 14 | 0.4 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 18 | 0.4 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 20 | 0.4 |
| (2,3677) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HA | 4 | 0.4 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 7 | 0.4 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 8 | 0.4 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 9 | 0.4 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 14 | 0.4 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 16 | 0.4 |
| (2,3666) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 1 | 0.4 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 2 | 0.4 |
| (2,3666) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 5 | 0.4 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 9 | 0.4 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 11 | 0.4 |
| (2,3666) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 15 | 0.4 |
| (2,3544) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 6 | 0.4 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 14 | 0.4 |
| (2,3539) | 1:32:A:ALA:HB1 | 1:32:A:ALA:HA | 5 | 0.4 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 1 | 0.4 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 14 | 0.4 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 18 | 0.4 |
| (2,3474) | 1:146:A:VAL:HG12 | 1:96:A:VAL:HA | 14 | 0.4 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 4 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 17 | 0.4 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 2 | 0.4 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 6 | 0.4 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 14 | 0.4 |
| (2,3390) | 1:56:A:ILE:HG23 | 1:65:A:PHE:HE1 | 9 | 0.4 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 11 | 0.4 |
| (2,3346) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 16 | 0.4 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 7 | 0.4 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 12 | 0.4 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 13 | 0.4 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 18 | 0.4 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 4 | 0.4 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD23 | 14 | 0.4 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 13 | 0.4 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 3 | 0.4 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 4 | 0.4 |
| (2,2425) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 20 | 0.4 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 6 | 0.4 |
| (2,2376) | 1:95:A:ALA:HB2 | 1:149:A:LYS:H | 7 | 0.4 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG23 | 16 | 0.4 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 8 | 0.4 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 2 | 0.4 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 7 | 0.4 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 13 | 0.4 |
| (2,1861) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 5 | 0.4 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG22 | 1 | 0.4 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 7 | 0.4 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 19 | 0.4 |
| (2,1831) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 10 | 0.4 |
| (2,1827) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HG | 4 | 0.4 |
| (2,1824) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 11 | 0.4 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 11 | 0.4 |
| (2,1807) | 1:151:A:MET:HE3 | 1:174:A:GLU:HG2 | 5 | 0.4 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 10 | 0.4 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 17 | 0.4 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 19 | 0.4 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 7 | 0.4 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG21 | 16 | 0.4 |
| (2,1699) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 1 | 0.4 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 2 | 0.4 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 3 | 0.4 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 4 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1699) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 5 | 0.4 |
| (2,1699) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 10 | 0.4 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 13 | 0.4 |
| (2,1699) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 15 | 0.4 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 7 | 0.4 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 10 | 0.4 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 12 | 0.4 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 9 | 0.4 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 20 | 0.4 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 18 | 0.4 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 20 | 0.4 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 3 | 0.4 |
| (2,1221) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 5 | 0.4 |
| (2,1221) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 6 | 0.4 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 8 | 0.4 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 20 | 0.4 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 5 | 0.4 |
| (2,1156) | 1:144:A:LEU:HD21 | 1:106:A:PHE:HE1 | 9 | 0.4 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 3 | 0.4 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 4 | 0.4 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 17 | 0.4 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 18 | 0.4 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 7 | 0.4 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 14 | 0.4 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 12 | 0.4 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD12 | 18 | 0.4 |
| (2,521) | 1:129:A:THR:HG22 | 1:129:A:THR:H | 11 | 0.4 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 17 | 0.4 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 20 | 0.4 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 4 | 0.4 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 7 | 0.4 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 13 | 0.4 |
| (2,405) | 1:95:A:ALA:HB2 | 1:149:A:LYS:H | 19 | 0.4 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 3 | 0.4 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 13 | 0.4 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 19 | 0.4 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 17 | 0.4 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 10 | 0.4 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 13 | 0.4 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 18 | 0.4 |
| (2,29) | 1:88:A:TYR:HD1 | 1:159:A:TYR:HD1 | 20 | 0.4 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 19 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 10 | 0.39 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 9 | 0.39 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD12 | 6 | 0.39 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 5 | 0.39 |
| (4,368) | 1:20:A:ALA:HB2 | 1:22:A:ILE:HB | 15 | 0.39 |
| (4,292) | 1:122:A:VAL:HG23 | 1:118:A:SER:H | 16 | 0.39 |
| (4,259) | 1:117:A:MET:HE3 | 2:201:A:NAD:H2A | 13 | 0.39 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD11 | 9 | 0.39 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 18 | 0.39 |
| (4,34) | 1:24:A:LEU:H | 1:22:A:ILE:HD13 | 19 | 0.39 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD23 | 18 | 0.39 |
| (2,3863) | 1:24:A:LEU:HA | 1:24:A:LEU:HD21 | 1 | 0.39 |
| (2,3847) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 14 | 0.39 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 17 | 0.39 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 2 | 0.39 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 7 | 0.39 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 13 | 0.39 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 17 | 0.39 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 3 | 0.39 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 9 | 0.39 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 11 | 0.39 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD12 | 12 | 0.39 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 18 | 0.39 |
| (2,3798) | 1:48:A:ILE:HD13 | 1:48:A:ILE:HG13 | 4 | 0.39 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 1 | 0.39 |
| (2,3781) | 1:142:A:VAL:HG11 | 1:142:A:VAL:HB | 3 | 0.39 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 6 | 0.39 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 17 | 0.39 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 1 | 0.39 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 3 | 0.39 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 6 | 0.39 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 8 | 0.39 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 10 | 0.39 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 3 | 0.39 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 6 | 0.39 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 17 | 0.39 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 3 | 0.39 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 4 | 0.39 |
| (2,3666) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 10 | 0.39 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 12 | 0.39 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 13 | 0.39 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 14 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3607) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 2 | 0.39 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 12 | 0.39 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 16 | 0.39 |
| (2,3527) | 1:84:A:VAL:HG21 | 1:85:A:ASP:HB2 | 11 | 0.39 |
| (2,3484) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 8 | 0.39 |
| (2,3467) | 1:11:A:LEU:HD12 | 1:38:A:LEU:HA | 10 | 0.39 |
| (2,3428) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 2 | 0.39 |
| (2,3409) | 1:84:A:VAL:HG11 | 1:85:A:ASP:H | 7 | 0.39 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 10 | 0.39 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 11 | 0.39 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 15 | 0.39 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 19 | 0.39 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 14 | 0.39 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 9 | 0.39 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 9 | 0.39 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 16 | 0.39 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 15 | 0.39 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 19 | 0.39 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 19 | 0.39 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 1 | 0.39 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 14 | 0.39 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 1 | 0.39 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 15 | 0.39 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 17 | 0.39 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 8 | 0.39 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 4 | 0.39 |
| (2,1872) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 7 | 0.39 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 17 | 0.39 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 20 | 0.39 |
| (2,1827) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HG | 11 | 0.39 |
| (2,1827) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HG | 12 | 0.39 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 7 | 0.39 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 10 | 0.39 |
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 9 | 0.39 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 12 | 0.39 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 4 | 0.39 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 7 | 0.39 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 12 | 0.39 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 16 | 0.39 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 6 | 0.39 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 10 | 0.39 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 1 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 3 | 0.39 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 4 | 0.39 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 20 | 0.39 |
| (2,1720) | 1:86:A:LEU:HA | 1:84:A:VAL:HG13 | 1 | 0.39 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 12 | 0.39 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 14 | 0.39 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB2 | 19 | 0.39 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB2 | 20 | 0.39 |
| (2,1692) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 3 | 0.39 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 8 | 0.39 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 4 | 0.39 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 3 | 0.39 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 18 | 0.39 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 18 | 0.39 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 3 | 0.39 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 10 | 0.39 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 7 | 0.39 |
| (2,1377) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 13 | 0.39 |
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 8 | 0.39 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 2 | 0.39 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 11 | 0.39 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 14 | 0.39 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 17 | 0.39 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 18 | 0.39 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 19 | 0.39 |
| (2,1211) | 1:177:A:LYS:HD2 | 1:177:A:LYS:HA | 9 | 0.39 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 10 | 0.39 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 4 | 0.39 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 7 | 0.39 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 9 | 0.39 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 10 | 0.39 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 3 | 0.39 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 10 | 0.39 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 11 | 0.39 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 16 | 0.39 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 15 | 0.39 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 7 | 0.39 |
| (2,708) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 6 | 0.39 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 5 | 0.39 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 10 | 0.39 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 15 | 0.39 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 2 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 7 | 0.39 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 16 | 0.39 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 3 | 0.39 |
| (2,454) | 1:35:A:LYS:HB2 | 1:35:A:LYS:H | 20 | 0.39 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 18 | 0.39 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 9 | 0.39 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 16 | 0.39 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 17 | 0.39 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 5 | 0.39 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 7 | 0.39 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 4 | 0.39 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 9 | 0.39 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 14 | 0.39 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 9 | 0.39 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 11 | 0.38 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 8 | 0.38 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 19 | 0.38 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 11 | 0.38 |
| (4,379) | 1:50:A:MET:HA | 1:39:A:ALA:HB3 | 3 | 0.38 |
| (4,364) | 1:4:A:MET:HE2 | 1:58:A:GLU:HG3 | 17 | 0.38 |
| (4,299) | 1:168:A:ILE:HD12 | 1:96:A:VAL:HA | 7 | 0.38 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 12 | 0.38 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 11 | 0.38 |
| (4,208) | 1:14:A:VAL:HG21 | 1:11:A:LEU:HA | 20 | 0.38 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 6 | 0.38 |
| (4,15) | 1:177:A:LYS:H | 1:110:A:LEU:HD13 | 18 | 0.38 |
| (4,6) | 1:65:A:PHE:HE1 | 1:74:A:ILE:HG23 | 5 | 0.38 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD22 | 17 | 0.38 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD23 | 8 | 0.38 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 15 | 0.38 |
| (2,3964) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H6N | 4 | 0.38 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 13 | 0.38 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 20 | 0.38 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD22 | 18 | 0.38 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 6 | 0.38 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 6 | 0.38 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 17 | 0.38 |
| (2,3791) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 5 | 0.38 |
| (2,3790) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE3 | 7 | 0.38 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 14 | 0.38 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 10 | 0.38 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 15 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 20 | 0.38 |
| (2,3769) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 2 | 0.38 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 8 | 0.38 |
| (2,3769) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 12 | 0.38 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 15 | 0.38 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 18 | 0.38 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 4 | 0.38 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 1 | 0.38 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 5 | 0.38 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 1 | 0.38 |
| (2,3677) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HA | 12 | 0.38 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 15 | 0.38 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 6 | 0.38 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB2 | 7 | 0.38 |
| (2,3666) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 16 | 0.38 |
| (2,3666) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 17 | 0.38 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB2 | 19 | 0.38 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB2 | 20 | 0.38 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 15 | 0.38 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 20 | 0.38 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 17 | 0.38 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 8 | 0.38 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 18 | 0.38 |
| (2,3439) | 1:110:A:LEU:HD13 | 1:110:A:LEU:H | 9 | 0.38 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 16 | 0.38 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 17 | 0.38 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 4 | 0.38 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 6 | 0.38 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 15 | 0.38 |
| (2,3182) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 20 | 0.38 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD23 | 15 | 0.38 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 10 | 0.38 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 3 | 0.38 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 2 | 0.38 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 9 | 0.38 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 17 | 0.38 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 18 | 0.38 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 1 | 0.38 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG23 | 11 | 0.38 |
| (2,1859) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 13 | 0.38 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 17 | 0.38 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 4 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 5 | 0.38 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 7 | 0.38 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 16 | 0.38 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 6 | 0.38 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 5 | 0.38 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD13 | 16 | 0.38 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 8 | 0.38 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 9 | 0.38 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 11 | 0.38 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 13 | 0.38 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 14 | 0.38 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 19 | 0.38 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 20 | 0.38 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD21 | 7 | 0.38 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 13 | 0.38 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 16 | 0.38 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 7 | 0.38 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 8 | 0.38 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 10 | 0.38 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 14 | 0.38 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 4 | 0.38 |
| (2,1750) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 18 | 0.38 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 17 | 0.38 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 6 | 0.38 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB2 | 7 | 0.38 |
| (2,1699) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 16 | 0.38 |
| (2,1699) | 1:43:A:ALA:HB1 | 1:43:A:ALA:HA | 17 | 0.38 |
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 4 | 0.38 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 8 | 0.38 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 8 | 0.38 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 19 | 0.38 |
| (2,1546) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 16 | 0.38 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 19 | 0.38 |
| (2,1541) | 1:143:A:VAL:HG13 | 1:132:A:ARG:HA | 20 | 0.38 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 2 | 0.38 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 6 | 0.38 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 12 | 0.38 |
| (2,1534) | 1:151:A:MET:HE2 | 1:151:A:MET:HA | 1 | 0.38 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 4 | 0.38 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 6 | 0.38 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 10 | 0.38 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 15 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 4 | 0.38 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 8 | 0.38 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 1 | 0.38 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 16 | 0.38 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 14 | 0.38 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 8 | 0.38 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 10 | 0.38 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 1 | 0.38 |
| (2,1221) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 4 | 0.38 |
| (2,1221) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 10 | 0.38 |
| (2,1221) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 15 | 0.38 |
| (2,1221) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 16 | 0.38 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 14 | 0.38 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 15 | 0.38 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 9 | 0.38 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 20 | 0.38 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 1 | 0.38 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD13 | 18 | 0.38 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 18 | 0.38 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 16 | 0.38 |
| (2,584) | 1:17:A:HIS:H | 1:17:A:HIS:HD2 | 14 | 0.38 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 4 | 0.38 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 8 | 0.38 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 13 | 0.38 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 14 | 0.38 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 3 | 0.38 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 16 | 0.38 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 12 | 0.38 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 10 | 0.38 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 7 | 0.38 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 10 | 0.38 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 18 | 0.38 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 8 | 0.38 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 18 | 0.38 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 19 | 0.38 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 7 | 0.38 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 3 | 0.38 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 18 | 0.38 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 19 | 0.38 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 12 | 0.38 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 17 | 0.38 |
| (4,447) | 1:53:A:LEU:HD12 | 1:11:A:LEU:HD23 | 5 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 4 | 0.37 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 11 | 0.37 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 7 | 0.37 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 8 | 0.37 |
| (4,415) | 1:19:A:PRO:HB3 | 1:36:A:GLU:HG2 | 9 | 0.37 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 10 | 0.37 |
| (4,167) | 1:34:A:VAL:H | 1:11:A:LEU:HB3 | 5 | 0.37 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB2 | 13 | 0.37 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 13 | 0.37 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 14 | 0.37 |
| (2,3833) | 1:168:A:ILE:HD11 | 1:168:A:ILE:HG13 | 5 | 0.37 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 5 | 0.37 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 13 | 0.37 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 1 | 0.37 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 3 | 0.37 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 8 | 0.37 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 14 | 0.37 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 2 | 0.37 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 12 | 0.37 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 15 | 0.37 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 18 | 0.37 |
| (2,3759) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HB2 | 6 | 0.37 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 13 | 0.37 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 10 | 0.37 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 11 | 0.37 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 9 | 0.37 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG21 | 4 | 0.37 |
| (2,3666) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 8 | 0.37 |
| (2,3544) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 3 | 0.37 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 16 | 0.37 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 4 | 0.37 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 15 | 0.37 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 16 | 0.37 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 17 | 0.37 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 11 | 0.37 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 19 | 0.37 |
| (2,3459) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 18 | 0.37 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 12 | 0.37 |
| (2,3346) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 13 | 0.37 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 14 | 0.37 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 14 | 0.37 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 5 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 5 | 0.37 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 4 | 0.37 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 15 | 0.37 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 5 | 0.37 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 3 | 0.37 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 2 | 0.37 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 6 | 0.37 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 7 | 0.37 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 10 | 0.37 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD12 | 12 | 0.37 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 12 | 0.37 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 20 | 0.37 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 5 | 0.37 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 17 | 0.37 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 20 | 0.37 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 1 | 0.37 |
| (2,1838) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 15 | 0.37 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 16 | 0.37 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 17 | 0.37 |
| (2,1819) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HG | 14 | 0.37 |
| (2,1819) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HG | 19 | 0.37 |
| (2,1796) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD12 | 16 | 0.37 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 12 | 0.37 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 1 | 0.37 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 3 | 0.37 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 5 | 0.37 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 12 | 0.37 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 14 | 0.37 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 17 | 0.37 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 20 | 0.37 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 13 | 0.37 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 20 | 0.37 |
| (2,1699) | 1:43:A:ALA:HA | 1:43:A:ALA:HB3 | 8 | 0.37 |
| (2,1692) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 10 | 0.37 |
| (2,1692) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 11 | 0.37 |
| (2,1692) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 13 | 0.37 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 16 | 0.37 |
| (2,1599) | 1:4:A:MET:HE2 | 1:52:A:GLU:HA | 19 | 0.37 |
| (2,1546) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 7 | 0.37 |
| (2,1541) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 17 | 0.37 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 8 | 0.37 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 15 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 8 | 0.37 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 9 | 0.37 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 11 | 0.37 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 13 | 0.37 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 14 | 0.37 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 19 | 0.37 |
| (2,1514) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 8 | 0.37 |
| (2,1509) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 8 | 0.37 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 19 | 0.37 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 11 | 0.37 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 1 | 0.37 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 5 | 0.37 |
| (2,1380) | 1:9:A:LYS:HB2 | 1:65:A:PHE:HE1 | 10 | 0.37 |
| (2,1288) | 1:167:A:LEU:HD23 | 1:167:A:LEU:HA | 13 | 0.37 |
| (2,1221) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 12 | 0.37 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 13 | 0.37 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 1 | 0.37 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 3 | 0.37 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 7 | 0.37 |
| (2,874) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE21 | 7 | 0.37 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 3 | 0.37 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 12 | 0.37 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 13 | 0.37 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 11 | 0.37 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 9 | 0.37 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 1 | 0.37 |
| (2,521) | 1:129:A:THR:HG23 | 1:129:A:THR:H | 7 | 0.37 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 12 | 0.37 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 15 | 0.37 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 7 | 0.37 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 11 | 0.37 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 18 | 0.37 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 9 | 0.37 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 11 | 0.37 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 5 | 0.37 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 9 | 0.37 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 10 | 0.37 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 14 | 0.37 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 15 | 0.37 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 1 | 0.37 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 4 | 0.37 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 6 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 13 | 0.37 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 3 | 0.37 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 4 | 0.37 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 5 | 0.37 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 6 | 0.37 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 15 | 0.37 |
| (4,451) | 1:168:A:ILE:HD11 | 1:168:A:ILE:HG12 | 12 | 0.36 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 7 | 0.36 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 12 | 0.36 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 7 | 0.36 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 14 | 0.36 |
| (4,432) | 1:131:A:ALA:HB1 | 1:128:A:ILE:HB | 6 | 0.36 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 1 | 0.36 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 3 | 0.36 |
| (4,319) | 1:26:A:LEU:HD22 | 1:14:A:VAL:HA | 19 | 0.36 |
| (4,300) | 1:97:A:LEU:HD23 | 1:156:A:PHE:HB3 | 7 | 0.36 |
| (4,299) | 1:168:A:ILE:HD12 | 1:152:A:ALA:HA | 1 | 0.36 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 18 | 0.36 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 8 | 0.36 |
| (4,70) | 1:130:A:THR:H | 2:201:A:NAD:H4D | 14 | 0.36 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 16 | 0.36 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 3 | 0.36 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD23 | 14 | 0.36 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 14 | 0.36 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 18 | 0.36 |
| (2,3826) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB3 | 10 | 0.36 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD21 | 15 | 0.36 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 10 | 0.36 |
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 10 | 0.36 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 18 | 0.36 |
| (2,3794) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HB | 20 | 0.36 |
| (2,3791) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 13 | 0.36 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 6 | 0.36 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 7 | 0.36 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 8 | 0.36 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 9 | 0.36 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 5 | 0.36 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 6 | 0.36 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 8 | 0.36 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 9 | 0.36 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 12 | 0.36 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 14 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 1 | 0.36 |
| (2,3769) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 7 | 0.36 |
| (2,3769) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 9 | 0.36 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 9 | 0.36 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 20 | 0.36 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 9 | 0.36 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 20 | 0.36 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 12 | 0.36 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 3 | 0.36 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 16 | 0.36 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 19 | 0.36 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 6 | 0.36 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 13 | 0.36 |
| (2,3659) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 3 | 0.36 |
| (2,3600) | 1:42:A:LYS:HE3 | 1:39:A:ALA:HA | 15 | 0.36 |
| (2,3544) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 5 | 0.36 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 3 | 0.36 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 7 | 0.36 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 9 | 0.36 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 12 | 0.36 |
| (2,3371) | 1:20:A:ALA:HB2 | 1:18:A:ASN:HD21 | 3 | 0.36 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 10 | 0.36 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 2 | 0.36 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 5 | 0.36 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 13 | 0.36 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 18 | 0.36 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD21 | 5 | 0.36 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD23 | 10 | 0.36 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 18 | 0.36 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 8 | 0.36 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 9 | 0.36 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 10 | 0.36 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 14 | 0.36 |
| (2,2748) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 20 | 0.36 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 20 | 0.36 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 7 | 0.36 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 10 | 0.36 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 18 | 0.36 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 17 | 0.36 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 8 | 0.36 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 18 | 0.36 |
| (2,1874) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 13 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 1 | 0.36 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 3 | 0.36 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 14 | 0.36 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 15 | 0.36 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 4 | 0.36 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 17 | 0.36 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 8 | 0.36 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 9 | 0.36 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 13 | 0.36 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 9 | 0.36 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 10 | 0.36 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 4 | 0.36 |
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 2 | 0.36 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 4 | 0.36 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD21 | 8 | 0.36 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 9 | 0.36 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 10 | 0.36 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 11 | 0.36 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 15 | 0.36 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 3 | 0.36 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 6 | 0.36 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 15 | 0.36 |
| (2,1750) | 1:158:A:PHE:HB2 | 1:168:A:ILE:HG12 | 17 | 0.36 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 11 | 0.36 |
| (2,1555) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 20 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HB2 | 1 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 2 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 4 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 9 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HB2 | 11 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 12 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 13 | 0.36 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 15 | 0.36 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 9 | 0.36 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 16 | 0.36 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 3 | 0.36 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 10 | 0.36 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 2 | 0.36 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 7 | 0.36 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 17 | 0.36 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 14 | 0.36 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 16 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 2 | 0.36 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 12 | 0.36 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 20 | 0.36 |
| (2,1276) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HE1 | 4 | 0.36 |
| (2,1221) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 9 | 0.36 |
| (2,1211) | 1:177:A:LYS:HD2 | 1:177:A:LYS:HA | 2 | 0.36 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 2 | 0.36 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 18 | 0.36 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 9 | 0.36 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 20 | 0.36 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 10 | 0.36 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD13 | 17 | 0.36 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 5 | 0.36 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 16 | 0.36 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 19 | 0.36 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 15 | 0.36 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 17 | 0.36 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 19 | 0.36 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 5 | 0.36 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 9 | 0.36 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 9 | 0.36 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 9 | 0.36 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 8 | 0.36 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 12 | 0.36 |
| (2,379) | 1:156:A:PHE:H | 1:168:A:ILE:HD11 | 5 | 0.36 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 2 | 0.36 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 12 | 0.36 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 17 | 0.36 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 6 | 0.36 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 20 | 0.36 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD23 | 7 | 0.36 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 6 | 0.36 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 13 | 0.36 |
| (2,175) | 1:53:A:LEU:HD21 | 1:56:A:ILE:H | 2 | 0.36 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 10 | 0.36 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 11 | 0.36 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 5 | 0.36 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 7 | 0.36 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 12 | 0.36 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 14 | 0.36 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 19 | 0.36 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 15 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 17 | 0.36 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 6 | 0.36 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 19 | 0.35 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 9 | 0.35 |
| (4,438) | 1:108:A:LEU:HG | 1:108:A:LEU:HD13 | 16 | 0.35 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 6 | 0.35 |
| (4,430) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB3 | 18 | 0.35 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 9 | 0.35 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 3 | 0.35 |
| (4,338) | 1:111:A:LYS:HD3 | 1:104:A:LYS:HA | 15 | 0.35 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 1 | 0.35 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 8 | 0.35 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 13 | 0.35 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 9 | 0.35 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 10 | 0.35 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 11 | 0.35 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 12 | 0.35 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 4 | 0.35 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 8 | 0.35 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 10 | 0.35 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD21 | 6 | 0.35 |
| (2,3822) | 1:53:A:LEU:HD13 | 1:53:A:LEU:HD22 | 10 | 0.35 |
| (2,3822) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HD22 | 17 | 0.35 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 6 | 0.35 |
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 7 | 0.35 |
| (2,3789) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HB3 | 3 | 0.35 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 2 | 0.35 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 9 | 0.35 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 11 | 0.35 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 14 | 0.35 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 17 | 0.35 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 18 | 0.35 |
| (2,3783) | 1:143:A:VAL:HG11 | 1:143:A:VAL:HB | 20 | 0.35 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 15 | 0.35 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 18 | 0.35 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 19 | 0.35 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 19 | 0.35 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 1 | 0.35 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 15 | 0.35 |
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 18 | 0.35 |
| (2,3677) | 1:15:A:LEU:HD22 | 1:15:A:LEU:HA | 20 | 0.35 |
| (2,3600) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 5 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3600) | 1:42:A:LYS:HE3 | 1:39:A:ALA:HA | 6 | 0.35 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 19 | 0.35 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 2 | 0.35 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 6 | 0.35 |
| (2,3484) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 10 | 0.35 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 10 | 0.35 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 12 | 0.35 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 8 | 0.35 |
| (2,3439) | 1:110:A:LEU:HD13 | 1:110:A:LEU:H | 5 | 0.35 |
| (2,3408) | 1:7:A:VAL:HG11 | 1:7:A:VAL:H | 5 | 0.35 |
| (2,3408) | 1:7:A:VAL:HG13 | 1:7:A:VAL:H | 20 | 0.35 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 1 | 0.35 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 16 | 0.35 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 1 | 0.35 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 12 | 0.35 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 20 | 0.35 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 3 | 0.35 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 12 | 0.35 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 12 | 0.35 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 3 | 0.35 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 11 | 0.35 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 20 | 0.35 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 8 | 0.35 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 19 | 0.35 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 11 | 0.35 |
| (2,1874) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 1 | 0.35 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD12 | 5 | 0.35 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 16 | 0.35 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 19 | 0.35 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 20 | 0.35 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 13 | 0.35 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 19 | 0.35 |
| (2,1850) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD23 | 4 | 0.35 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD12 | 12 | 0.35 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 10 | 0.35 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 10 | 0.35 |
| (2,1838) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 18 | 0.35 |
| (2,1832) | 1:53:A:LEU:HD22 | 1:56:A:ILE:HB | 6 | 0.35 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 14 | 0.35 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 17 | 0.35 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 18 | 0.35 |
| (2,1819) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HG | 16 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 9 | 0.35 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 1 | 0.35 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 3 | 0.35 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 5 | 0.35 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 2 | 0.35 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 5 | 0.35 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 2 | 0.35 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 16 | 0.35 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 15 | 0.35 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 9 | 0.35 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 11 | 0.35 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 19 | 0.35 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 1 | 0.35 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 10 | 0.35 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 2 | 0.35 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 4 | 0.35 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 7 | 0.35 |
| (2,1692) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 12 | 0.35 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 14 | 0.35 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 18 | 0.35 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 6 | 0.35 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 10 | 0.35 |
| (2,1541) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 14 | 0.35 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 7 | 0.35 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 11 | 0.35 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 13 | 0.35 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 4 | 0.35 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 6 | 0.35 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 12 | 0.35 |
| (2,1459) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 7 | 0.35 |
| (2,1412) | 1:66:A:ALA:HB2 | 1:31:A:TRP:HZ3 | 18 | 0.35 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 5 | 0.35 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 20 | 0.35 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 3 | 0.35 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 5 | 0.35 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 18 | 0.35 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 1 | 0.35 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 4 | 0.35 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 5 | 0.35 |
| (2,1274) | 1:160:A:LEU:HD21 | 1:91:A:GLN:HE22 | 15 | 0.35 |
| (2,1257) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 10 | 0.35 |
| (2,1211) | 1:177:A:LYS:HD2 | 1:177:A:LYS:HA | 7 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1201) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 7 | 0.35 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 12 | 0.35 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 17 | 0.35 |
| (2,1201) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 20 | 0.35 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 15 | 0.35 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 19 | 0.35 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 20 | 0.35 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 1 | 0.35 |
| (2,775) | 1:87:A:GLY:H | 1:81:A:SER:HA | 10 | 0.35 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 15 | 0.35 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 4 | 0.35 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB2 | 19 | 0.35 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 4 | 0.35 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 11 | 0.35 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 14 | 0.35 |
| (2,521) | 1:129:A:THR:HG23 | 1:129:A:THR:H | 3 | 0.35 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 18 | 0.35 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 14 | 0.35 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 13 | 0.35 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 4 | 0.35 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 19 | 0.35 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 4 | 0.35 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 7 | 0.35 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 10 | 0.35 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 11 | 0.35 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 2 | 0.35 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 3 | 0.35 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 8 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 2 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 8 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 9 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 11 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 13 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 15 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 17 | 0.35 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 20 | 0.35 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 8 | 0.35 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 14 | 0.35 |
| (2,19) | 1:13:A:LEU:HA | 1:17:A:HIS:HD2 | 2 | 0.35 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 4 | 0.35 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 14 | 0.34 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 16 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 1 | 0.34 |
| (4,387) | 1:83:A:GLU:HA | 1:82:A:VAL:HG12 | 4 | 0.34 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 14 | 0.34 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 17 | 0.34 |
| (4,379) | 1:50:A:MET:HA | 1:39:A:ALA:HB3 | 12 | 0.34 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 7 | 0.34 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 13 | 0.34 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 12 | 0.34 |
| (4,325) | 1:7:A:VAL:HG11 | 1:10:A:PHE:HB3 | 11 | 0.34 |
| (4,292) | 1:122:A:VAL:HG23 | 1:118:A:SER:H | 6 | 0.34 |
| (4,244) | 1:51:A:GLU:HG2 | 1:72:A:GLU:H | 1 | 0.34 |
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 1 | 0.34 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 17 | 0.34 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 1 | 0.34 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD23 | 17 | 0.34 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD23 | 3 | 0.34 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 7 | 0.34 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 19 | 0.34 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 12 | 0.34 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 14 | 0.34 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 13 | 0.34 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 15 | 0.34 |
| (2,3804) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG21 | 20 | 0.34 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 3 | 0.34 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 3 | 0.34 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 8 | 0.34 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 12 | 0.34 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 20 | 0.34 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 2 | 0.34 |
| (2,3783) | 1:143:A:VAL:HG11 | 1:143:A:VAL:HB | 4 | 0.34 |
| (2,3783) | 1:143:A:VAL:HG11 | 1:143:A:VAL:HB | 8 | 0.34 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 15 | 0.34 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 18 | 0.34 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 17 | 0.34 |
| (2,3772) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 15 | 0.34 |
| (2,3759) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HB2 | 18 | 0.34 |
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD22 | 3 | 0.34 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD21 | 7 | 0.34 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 13 | 0.34 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 2 | 0.34 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 8 | 0.34 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 12 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3677) | 1:15:A:LEU:HD21 | 1:15:A:LEU:HA | 10 | 0.34 |
| (2,3659) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 10 | 0.34 |
| (2,3659) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 11 | 0.34 |
| (2,3659) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 13 | 0.34 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 16 | 0.34 |
| (2,3600) | 1:42:A:LYS:HE3 | 1:39:A:ALA:HA | 17 | 0.34 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 16 | 0.34 |
| (2,3484) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 6 | 0.34 |
| (2,3484) | 1:124:A:LEU:HD12 | 1:167:A:LEU:HA | 9 | 0.34 |
| (2,3484) | 1:124:A:LEU:HD12 | 1:167:A:LEU:HA | 15 | 0.34 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 6 | 0.34 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 20 | 0.34 |
| (2,3459) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 10 | 0.34 |
| (2,3439) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 10 | 0.34 |
| (2,3428) | 1:108:A:LEU:HD13 | 2:201:A:NAD:H2A | 18 | 0.34 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 10 | 0.34 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 15 | 0.34 |
| (2,3391) | 1:56:A:ILE:HG21 | 1:65:A:PHE:HD1 | 14 | 0.34 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 12 | 0.34 |
| (2,3384) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HD22 | 1 | 0.34 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 10 | 0.34 |
| (2,3288) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 10 | 0.34 |
| (2,3274) | 1:57:A:VAL:HG13 | 1:66:A:ALA:HA | 5 | 0.34 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 18 | 0.34 |
| (2,3248) | 1:160:A:LEU:HD21 | 1:91:A:GLN:HE22 | 15 | 0.34 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 3 | 0.34 |
| (2,3196) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 6 | 0.34 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 7 | 0.34 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 20 | 0.34 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 8 | 0.34 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 2 | 0.34 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 18 | 0.34 |
| (2,3156) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 2 | 0.34 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD23 | 6 | 0.34 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 8 | 0.34 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD23 | 11 | 0.34 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 12 | 0.34 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 2 | 0.34 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 6 | 0.34 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 7 | 0.34 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 18 | 0.34 |
| (2,2376) | 1:95:A:ALA:HB2 | 1:149:A:LYS:H | 19 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 9 | 0.34 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 1 | 0.34 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 2 | 0.34 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 3 | 0.34 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 2 | 0.34 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 14 | 0.34 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 5 | 0.34 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 16 | 0.34 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 4 | 0.34 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 7 | 0.34 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 16 | 0.34 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 7 | 0.34 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 12 | 0.34 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 17 | 0.34 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 20 | 0.34 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 8 | 0.34 |
| (2,1869) | 1:97:A:LEU:HD22 | 1:96:A:VAL:HB | 10 | 0.34 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 7 | 0.34 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 3 | 0.34 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 7 | 0.34 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 9 | 0.34 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD23 | 18 | 0.34 |
| (2,1850) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD23 | 19 | 0.34 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 14 | 0.34 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 4 | 0.34 |
| (2,1838) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 2 | 0.34 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 12 | 0.34 |
| (2,1838) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 14 | 0.34 |
| (2,1838) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 20 | 0.34 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 5 | 0.34 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 8 | 0.34 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 13 | 0.34 |
| (2,1820) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 12 | 0.34 |
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 10 | 0.34 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 15 | 0.34 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 20 | 0.34 |
| (2,1804) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 2 | 0.34 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 8 | 0.34 |
| (2,1804) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 12 | 0.34 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 14 | 0.34 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 15 | 0.34 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 18 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 2 | 0.34 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD21 | 6 | 0.34 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 2 | 0.34 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 18 | 0.34 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 9 | 0.34 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 5 | 0.34 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 17 | 0.34 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 20 | 0.34 |
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 3 | 0.34 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE1 | 9 | 0.34 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 12 | 0.34 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 14 | 0.34 |
| (2,1563) | 1:48:A:ILE:HG22 | 1:53:A:LEU:HB2 | 3 | 0.34 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 5 | 0.34 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 8 | 0.34 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 14 | 0.34 |
| (2,1546) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 17 | 0.34 |
| (2,1546) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HB2 | 18 | 0.34 |
| (2,1546) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 20 | 0.34 |
| (2,1541) | 1:143:A:VAL:HG12 | 1:132:A:ARG:HA | 15 | 0.34 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 19 | 0.34 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 7 | 0.34 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 9 | 0.34 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 11 | 0.34 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 13 | 0.34 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 17 | 0.34 |
| (2,1531) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 16 | 0.34 |
| (2,1521) | 1:96:A:VAL:HG11 | 1:96:A:VAL:HA | 5 | 0.34 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 7 | 0.34 |
| (2,1405) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 10 | 0.34 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 16 | 0.34 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 15 | 0.34 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 20 | 0.34 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 12 | 0.34 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 2 | 0.34 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 3 | 0.34 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 7 | 0.34 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 9 | 0.34 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 13 | 0.34 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 14 | 0.34 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 15 | 0.34 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 17 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 20 | 0.34 |
| (2,1201) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 9 | 0.34 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 13 | 0.34 |
| (2,1201) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 16 | 0.34 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 2 | 0.34 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 17 | 0.34 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 15 | 0.34 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 19 | 0.34 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 11 | 0.34 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 3 | 0.34 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 5 | 0.34 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 16 | 0.34 |
| (2,567) | 1:88:A:TYR:H | 1:86:A:LEU:HB3 | 1 | 0.34 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 3 | 0.34 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 10 | 0.34 |
| (2,521) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 16 | 0.34 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 5 | 0.34 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 11 | 0.34 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 16 | 0.34 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 11 | 0.34 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 16 | 0.34 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 19 | 0.34 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 3 | 0.34 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 7 | 0.34 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 10 | 0.34 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 15 | 0.34 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 8 | 0.34 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 15 | 0.34 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 17 | 0.34 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 15 | 0.34 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 17 | 0.34 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 1 | 0.34 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 3 | 0.34 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 4 | 0.34 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 5 | 0.34 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 10 | 0.34 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 16 | 0.34 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 18 | 0.34 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 2 | 0.34 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 4 | 0.34 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 15 | 0.34 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 11 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 13 | 0.34 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 14 | 0.34 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 16 | 0.34 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 9 | 0.34 |
| (4,451) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG12 | 6 | 0.33 |
| (4,451) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG12 | 10 | 0.33 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 18 | 0.33 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 16 | 0.33 |
| (4,430) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 5 | 0.33 |
| (4,411) | 1:172:A:PRO:HB2 | 1:114:A:ILE:HG12 | 13 | 0.33 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 16 | 0.33 |
| (4,322) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 1 | 0.33 |
| (4,259) | 1:117:A:MET:HE3 | 2:201:A:NAD:H2A | 19 | 0.33 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 20 | 0.33 |
| (4,31) | 1:24:A:LEU:H | 1:24:A:LEU:HG | 20 | 0.33 |
| (2,3964) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H6N | 18 | 0.33 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 20 | 0.33 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 4 | 0.33 |
| (2,3833) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG13 | 7 | 0.33 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 3 | 0.33 |
| (2,3826) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB3 | 14 | 0.33 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 18 | 0.33 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 7 | 0.33 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 2 | 0.33 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 19 | 0.33 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 19 | 0.33 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 3 | 0.33 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 5 | 0.33 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 7 | 0.33 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 9 | 0.33 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 10 | 0.33 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD13 | 11 | 0.33 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 15 | 0.33 |
| (2,3785) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 15 | 0.33 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 1 | 0.33 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 10 | 0.33 |
| (2,3783) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 12 | 0.33 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 16 | 0.33 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 19 | 0.33 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 16 | 0.33 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 17 | 0.33 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 18 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3749) | 1:44:A:LYS:HG2 | 1:21:A:LEU:HD23 | 1 | 0.33 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 1 | 0.33 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 3 | 0.33 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 5 | 0.33 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 12 | 0.33 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 14 | 0.33 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 15 | 0.33 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 17 | 0.33 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 20 | 0.33 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 20 | 0.33 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG21 | 16 | 0.33 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 4 | 0.33 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 7 | 0.33 |
| (2,3659) | 1:20:A:ALA:HB1 | 1:20:A:ALA:HA | 12 | 0.33 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 14 | 0.33 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 18 | 0.33 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE2 | 14 | 0.33 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 20 | 0.33 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 3 | 0.33 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 5 | 0.33 |
| (2,3556) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 6 | 0.33 |
| (2,3556) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 12 | 0.33 |
| (2,3556) | 1:28:A:ALA:HB2 | 1:28:A:ALA:HA | 17 | 0.33 |
| (2,3502) | 1:21:A:LEU:HD11 | 1:14:A:VAL:HA | 3 | 0.33 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 2 | 0.33 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 15 | 0.33 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 4 | 0.33 |
| (2,3387) | 1:21:A:LEU:HD21 | 1:10:A:PHE:HE1 | 11 | 0.33 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 13 | 0.33 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 14 | 0.33 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 20 | 0.33 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 1 | 0.33 |
| (2,3196) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 5 | 0.33 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 8 | 0.33 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 11 | 0.33 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 14 | 0.33 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 17 | 0.33 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 19 | 0.33 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 7 | 0.33 |
| (2,3175) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 7 | 0.33 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 12 | 0.33 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 17 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3175) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 20 | 0.33 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD22 | 2 | 0.33 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD23 | 9 | 0.33 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD21 | 20 | 0.33 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD12 | 11 | 0.33 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 15 | 0.33 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD13 | 20 | 0.33 |
| (2,2738) | 1:30:A:GLY:H | 1:26:A:LEU:HD22 | 20 | 0.33 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 18 | 0.33 |
| (2,2308) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 16 | 0.33 |
| (2,2255) | 1:46:A:HIS:H | 1:22:A:ILE:HG23 | 5 | 0.33 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 17 | 0.33 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 1 | 0.33 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 2 | 0.33 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 9 | 0.33 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 12 | 0.33 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 13 | 0.33 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 14 | 0.33 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 20 | 0.33 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 3 | 0.33 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 9 | 0.33 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 14 | 0.33 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 20 | 0.33 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 6 | 0.33 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 4 | 0.33 |
| (2,1873) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 13 | 0.33 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 12 | 0.33 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 16 | 0.33 |
| (2,1863) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB3 | 10 | 0.33 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 3 | 0.33 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 7 | 0.33 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 10 | 0.33 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD23 | 13 | 0.33 |
| (2,1850) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD22 | 20 | 0.33 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 6 | 0.33 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 4 | 0.33 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 19 | 0.33 |
| (2,1819) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HG | 15 | 0.33 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 1 | 0.33 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 3 | 0.33 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 14 | 0.33 |
| (2,1807) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 19 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1804) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 7 | 0.33 |
| (2,1793) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 15 | 0.33 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 2 | 0.33 |
| (2,1758) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 4 | 0.33 |
| (2,1710) | 1:26:A:LEU:HD21 | 1:15:A:LEU:HA | 16 | 0.33 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 1 | 0.33 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 6 | 0.33 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 19 | 0.33 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 5 | 0.33 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 9 | 0.33 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 3 | 0.33 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 16 | 0.33 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 2 | 0.33 |
| (2,1549) | 1:37:A:LEU:HD13 | 1:41:A:MET:HG2 | 8 | 0.33 |
| (2,1534) | 1:151:A:MET:HA | 1:151:A:MET:HE1 | 13 | 0.33 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 2 | 0.33 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 19 | 0.33 |
| (2,1514) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 10 | 0.33 |
| (2,1509) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 18 | 0.33 |
| (2,1487) | 1:168:A:ILE:HD13 | 1:149:A:LYS:H | 5 | 0.33 |
| (2,1463) | 1:57:A:VAL:HG23 | 1:67:A:PHE:HE1 | 6 | 0.33 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 19 | 0.33 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 20 | 0.33 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 1 | 0.33 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 4 | 0.33 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 6 | 0.33 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 7 | 0.33 |
| (2,1405) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 11 | 0.33 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 14 | 0.33 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 20 | 0.33 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 5 | 0.33 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 8 | 0.33 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 15 | 0.33 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 6 | 0.33 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 8 | 0.33 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 11 | 0.33 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 12 | 0.33 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 16 | 0.33 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 19 | 0.33 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 8 | 0.33 |
| (2,1201) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 10 | 0.33 |
| (2,1201) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 14 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1201) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 15 | 0.33 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 5 | 0.33 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 8 | 0.33 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 10 | 0.33 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 13 | 0.33 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 19 | 0.33 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 10 | 0.33 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 14 | 0.33 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 18 | 0.33 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 14 | 0.33 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 1 | 0.33 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 11 | 0.33 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 2 | 0.33 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 17 | 0.33 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 4 | 0.33 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 1 | 0.33 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 8 | 0.33 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 2 | 0.33 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 5 | 0.33 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 9 | 0.33 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 15 | 0.33 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 17 | 0.33 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 8 | 0.33 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 11 | 0.33 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 14 | 0.33 |
| (2,175) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 1 | 0.33 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 2 | 0.33 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 7 | 0.33 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 16 | 0.33 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 20 | 0.33 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 9 | 0.33 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 12 | 0.33 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 6 | 0.33 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 15 | 0.33 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 17 | 0.33 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 6 | 0.33 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 11 | 0.32 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 8 | 0.32 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 3 | 0.32 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 4 | 0.32 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 16 | 0.32 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 20 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,218) | 1:172:A:PRO:HA | 1:106:A:PHE:HE1 | 9 | 0.32 |
| (4,208) | 1:14:A:VAL:HG22 | 1:11:A:LEU:HA | 18 | 0.32 |
| (4,70) | 1:130:A:THR:H | 2:201:A:NAD:H4D | 13 | 0.32 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 6 | 0.32 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 11 | 0.32 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 5 | 0.32 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 17 | 0.32 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 4 | 0.32 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 3 | 0.32 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 16 | 0.32 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 12 | 0.32 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 16 | 0.32 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 5 | 0.32 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 19 | 0.32 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 4 | 0.32 |
| (2,3813) | 1:56:A:ILE:HD13 | 1:11:A:LEU:HD11 | 2 | 0.32 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 8 | 0.32 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 1 | 0.32 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 13 | 0.32 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 14 | 0.32 |
| (2,3783) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 3 | 0.32 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 20 | 0.32 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 11 | 0.32 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 13 | 0.32 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 10 | 0.32 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 12 | 0.32 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 2 | 0.32 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 6 | 0.32 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 9 | 0.32 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 20 | 0.32 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD21 | 8 | 0.32 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 9 | 0.32 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 10 | 0.32 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD22 | 11 | 0.32 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 5 | 0.32 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 19 | 0.32 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 2 | 0.32 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 5 | 0.32 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 4 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 1 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 2 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 4 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 8 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB2 | 1:28:A:ALA:HA | 13 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 14 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 15 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 16 | 0.32 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 19 | 0.32 |
| (2,3502) | 1:21:A:LEU:HD11 | 1:14:A:VAL:HA | 1 | 0.32 |
| (2,3490) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HA | 1 | 0.32 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 13 | 0.32 |
| (2,3459) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 15 | 0.32 |
| (2,3387) | 1:21:A:LEU:HD21 | 1:10:A:PHE:HE1 | 4 | 0.32 |
| (2,3387) | 1:21:A:LEU:HD21 | 1:10:A:PHE:HE1 | 6 | 0.32 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 9 | 0.32 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 1 | 0.32 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 2 | 0.32 |
| (2,3196) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 4 | 0.32 |
| (2,3196) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 16 | 0.32 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 18 | 0.32 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 3 | 0.32 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 4 | 0.32 |
| (2,3175) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 9 | 0.32 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 13 | 0.32 |
| (2,3175) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 16 | 0.32 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 4 | 0.32 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 12 | 0.32 |
| (2,2198) | 1:21:A:LEU:HB2 | 1:21:A:LEU:H | 1 | 0.32 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 9 | 0.32 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 10 | 0.32 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 14 | 0.32 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 4 | 0.32 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 11 | 0.32 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 18 | 0.32 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 17 | 0.32 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 20 | 0.32 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 19 | 0.32 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 19 | 0.32 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 5 | 0.32 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 6 | 0.32 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 8 | 0.32 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 11 | 0.32 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 8 | 0.32 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 12 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 11 | 0.32 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 13 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD22 | 1 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD22 | 6 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 8 | 0.32 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD22 | 15 | 0.32 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 3 | 0.32 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD12 | 5 | 0.32 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 11 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 2 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 3 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 4 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 5 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 6 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 8 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 13 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 16 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 17 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 19 | 0.32 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 20 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 1 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 12 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG22 | 1:56:A:ILE:HG12 | 14 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 18 | 0.32 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 19 | 0.32 |
| (2,1838) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 1 | 0.32 |
| (2,1838) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 7 | 0.32 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 8 | 0.32 |
| (2,1838) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 11 | 0.32 |
| (2,1838) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 13 | 0.32 |
| (2,1833) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HB | 20 | 0.32 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 7 | 0.32 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 9 | 0.32 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 11 | 0.32 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 12 | 0.32 |
| (2,1832) | 1:53:A:LEU:HD22 | 1:56:A:ILE:HB | 16 | 0.32 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 20 | 0.32 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 13 | 0.32 |
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 5 | 0.32 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 6 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 8 | 0.32 |
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 9 | 0.32 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 12 | 0.32 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 1 | 0.32 |
| (2,1804) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HB | 9 | 0.32 |
| (2,1796) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD12 | 10 | 0.32 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 1 | 0.32 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 4 | 0.32 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 18 | 0.32 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 8 | 0.32 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 9 | 0.32 |
| (2,1692) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 15 | 0.32 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 4 | 0.32 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 15 | 0.32 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 19 | 0.32 |
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 13 | 0.32 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 20 | 0.32 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 6 | 0.32 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 9 | 0.32 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 13 | 0.32 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 19 | 0.32 |
| (2,1532) | 1:34:A:VAL:HG13 | 1:34:A:VAL:HA | 1 | 0.32 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 8 | 0.32 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 15 | 0.32 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 16 | 0.32 |
| (2,1514) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 6 | 0.32 |
| (2,1514) | 1:124:A:LEU:HD12 | 1:167:A:LEU:HA | 9 | 0.32 |
| (2,1514) | 1:124:A:LEU:HD12 | 1:167:A:LEU:HA | 15 | 0.32 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 8 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 2 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 3 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 12 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 13 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 17 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 18 | 0.32 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 19 | 0.32 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 3 | 0.32 |
| (2,1395) | 1:39:A:ALA:HB3 | 1:40:A:LYS:H | 13 | 0.32 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 19 | 0.32 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 2 | 0.32 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 16 | 0.32 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 19 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1201) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 1 | 0.32 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 4 | 0.32 |
| (2,1201) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 19 | 0.32 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 2 | 0.32 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 13 | 0.32 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 1 | 0.32 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 4 | 0.32 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 14 | 0.32 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 5 | 0.32 |
| (2,1053) | 1:74:A:ILE:H | 1:34:A:VAL:H | 13 | 0.32 |
| (2,1014) | 1:160:A:LEU:H | 1:89:A:GLU:H | 13 | 0.32 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD12 | 7 | 0.32 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 9 | 0.32 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 3 | 0.32 |
| (2,629) | 1:44:A:LYS:H | 1:42:A:LYS:HG3 | 17 | 0.32 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 8 | 0.32 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 3 | 0.32 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 17 | 0.32 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 19 | 0.32 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 10 | 0.32 |
| (2,267) | 1:21:A:LEU:H | 1:18:A:ASN:HD21 | 3 | 0.32 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 8 | 0.32 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 3 | 0.32 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 12 | 0.32 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 14 | 0.32 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 13 | 0.32 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 13 | 0.32 |
| (2,130) | 1:173:A:ALA:HB1 | 1:173:A:ALA:H | 6 | 0.32 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 20 | 0.32 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 3 | 0.32 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 8 | 0.32 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 10 | 0.32 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 18 | 0.32 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 15 | 0.32 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 3 | 0.31 |
| (4,451) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG12 | 5 | 0.31 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 16 | 0.31 |
| (4,451) | 1:168:A:ILE:HD12 | 1:168:A:ILE:HG12 | 20 | 0.31 |
| (4,443) | 1:48:A:ILE:HD12 | 1:38:A:LEU:HB2 | 12 | 0.31 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 11 | 0.31 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 11 | 0.31 |
| (4,379) | 1:50:A:MET:HA | 1:39:A:ALA:HB3 | 17 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 6 | 0.31 |
| (4,316) | 1:37:A:LEU:HD23 | 1:8:A:SER:HB2 | 1 | 0.31 |
| (4,311) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 7 | 0.31 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 10 | 0.31 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 14 | 0.31 |
| (4,167) | 1:34:A:VAL:H | 1:54:A:LYS:HD3 | 7 | 0.31 |
| (4,15) | 1:177:A:LYS:H | 1:96:A:VAL:HG21 | 5 | 0.31 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 9 | 0.31 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 16 | 0.31 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 5 | 0.31 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 7 | 0.31 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 8 | 0.31 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 11 | 0.31 |
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 3 | 0.31 |
| (2,3832) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 14 | 0.31 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 5 | 0.31 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 6 | 0.31 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 8 | 0.31 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 11 | 0.31 |
| (2,3826) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB3 | 6 | 0.31 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 18 | 0.31 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 11 | 0.31 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 15 | 0.31 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 2 | 0.31 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 1 | 0.31 |
| (2,3809) | 1:176:A:ILE:HB | 1:110:A:LEU:HD11 | 9 | 0.31 |
| (2,3804) | 1:128:A:ILE:HG23 | 1:129:A:THR:HG21 | 12 | 0.31 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 18 | 0.31 |
| (2,3785) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 3 | 0.31 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 13 | 0.31 |
| (2,3759) | 1:53:A:LEU:HD12 | 1:53:A:LEU:HB2 | 10 | 0.31 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 4 | 0.31 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 5 | 0.31 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 2 | 0.31 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 16 | 0.31 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 6 | 0.31 |
| (2,3679) | 1:97:A:LEU:HD21 | 1:97:A:LEU:HA | 9 | 0.31 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 6 | 0.31 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 17 | 0.31 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 19 | 0.31 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 20 | 0.31 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 20 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 9 | 0.31 |
| (2,3556) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 10 | 0.31 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 11 | 0.31 |
| (2,3556) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 18 | 0.31 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 20 | 0.31 |
| (2,3531) | 1:151:A:MET:HE2 | 1:175:A:PHE:HB3 | 5 | 0.31 |
| (2,3484) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 17 | 0.31 |
| (2,3479) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 8 | 0.31 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 9 | 0.31 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 19 | 0.31 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 2 | 0.31 |
| (2,3428) | 1:108:A:LEU:HD13 | 2:201:A:NAD:H2A | 6 | 0.31 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 11 | 0.31 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 13 | 0.31 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 2 | 0.31 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 2 | 0.31 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 7 | 0.31 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 15 | 0.31 |
| (2,3384) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HD22 | 3 | 0.31 |
| (2,3378) | 1:66:A:ALA:HB2 | 1:31:A:TRP:HZ3 | 18 | 0.31 |
| (2,3266) | 1:53:A:LEU:HD11 | 1:67:A:PHE:HE1 | 6 | 0.31 |
| (2,3266) | 1:53:A:LEU:HD11 | 1:67:A:PHE:HE1 | 10 | 0.31 |
| (2,3196) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 10 | 0.31 |
| (2,3196) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 12 | 0.31 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 13 | 0.31 |
| (2,3196) | 1:176:A:ILE:HG22 | 1:176:A:ILE:HB | 15 | 0.31 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 8 | 0.31 |
| (2,3175) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 10 | 0.31 |
| (2,3175) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 14 | 0.31 |
| (2,3175) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 15 | 0.31 |
| (2,2886) | 1:178:A:VAL:H | 1:144:A:LEU:HD23 | 3 | 0.31 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 11 | 0.31 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 6 | 0.31 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 17 | 0.31 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 6 | 0.31 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 2 | 0.31 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 5 | 0.31 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 6 | 0.31 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 10 | 0.31 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 13 | 0.31 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 19 | 0.31 |
| (2,1886) | 1:73:A:LYS:HG2 | 1:33:A:PRO:HB2 | 13 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 3 | 0.31 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 16 | 0.31 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 3 | 0.31 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 9 | 0.31 |
| (2,1874) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 14 | 0.31 |
| (2,1874) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 18 | 0.31 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 3 | 0.31 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 9 | 0.31 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 18 | 0.31 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 2 | 0.31 |
| (2,1858) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HD11 | 10 | 0.31 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 19 | 0.31 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 6 | 0.31 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 10 | 0.31 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 5 | 0.31 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 5 | 0.31 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD21 | 9 | 0.31 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD23 | 12 | 0.31 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 16 | 0.31 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 9 | 0.31 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 16 | 0.31 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 9 | 0.31 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 11 | 0.31 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 14 | 0.31 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 13 | 0.31 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 15 | 0.31 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 17 | 0.31 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 3 | 0.31 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 5 | 0.31 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 7 | 0.31 |
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 18 | 0.31 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 19 | 0.31 |
| (2,1796) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD12 | 2 | 0.31 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 8 | 0.31 |
| (2,1782) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 19 | 0.31 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 2 | 0.31 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 6 | 0.31 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 8 | 0.31 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 9 | 0.31 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 12 | 0.31 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 16 | 0.31 |
| (2,1715) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 1 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 15 | 0.31 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 18 | 0.31 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 3 | 0.31 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 5 | 0.31 |
| (2,1586) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 6 | 0.31 |
| (2,1586) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 12 | 0.31 |
| (2,1586) | 1:28:A:ALA:HB2 | 1:28:A:ALA:HA | 17 | 0.31 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 3 | 0.31 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 1 | 0.31 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 4 | 0.31 |
| (2,1573) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 7 | 0.31 |
| (2,1573) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 10 | 0.31 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 16 | 0.31 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 17 | 0.31 |
| (2,1563) | 1:48:A:ILE:HG23 | 1:53:A:LEU:HB2 | 12 | 0.31 |
| (2,1541) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 10 | 0.31 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 4 | 0.31 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 5 | 0.31 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 5 | 0.31 |
| (2,1532) | 1:34:A:VAL:HG13 | 1:34:A:VAL:HA | 18 | 0.31 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 20 | 0.31 |
| (2,1463) | 1:57:A:VAL:HG22 | 1:67:A:PHE:HE1 | 17 | 0.31 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 16 | 0.31 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 8 | 0.31 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 15 | 0.31 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 2 | 0.31 |
| (2,1395) | 1:39:A:ALA:HB3 | 1:40:A:LYS:H | 4 | 0.31 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 6 | 0.31 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 7 | 0.31 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 9 | 0.31 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 11 | 0.31 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 9 | 0.31 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 13 | 0.31 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 14 | 0.31 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 16 | 0.31 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 20 | 0.31 |
| (2,1288) | 1:167:A:LEU:HD22 | 1:167:A:LEU:HA | 15 | 0.31 |
| (2,1276) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HE1 | 14 | 0.31 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 8 | 0.31 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 10 | 0.31 |
| (2,1208) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 5 | 0.31 |
| (2,1201) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 5 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1201) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 11 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 1 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 4 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 5 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 6 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 10 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 12 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 14 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 15 | 0.31 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 20 | 0.31 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 7 | 0.31 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 12 | 0.31 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 15 | 0.31 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 16 | 0.31 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 18 | 0.31 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 20 | 0.31 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 13 | 0.31 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 18 | 0.31 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 14 | 0.31 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 14 | 0.31 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 8 | 0.31 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 2 | 0.31 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 6 | 0.31 |
| (2,629) | 1:44:A:LYS:H | 1:42:A:LYS:HG3 | 12 | 0.31 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 12 | 0.31 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 3 | 0.31 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 16 | 0.31 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 4 | 0.31 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 20 | 0.31 |
| (2,266) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 1 | 0.31 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 18 | 0.31 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 12 | 0.31 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 13 | 0.31 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 4 | 0.31 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 9 | 0.31 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 1 | 0.31 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 2 | 0.31 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 17 | 0.31 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 1 | 0.31 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 5 | 0.31 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 16 | 0.31 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 19 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 20 | 0.31 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 3 | 0.31 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 8 | 0.31 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 12 | 0.31 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 15 | 0.31 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 18 | 0.31 |
| (2,32) | 1:88:A:TYR:HE1 | 1:159:A:TYR:HD1 | 12 | 0.31 |
| (2,21) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 15 | 0.31 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 2 | 0.31 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 12 | 0.31 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 14 | 0.31 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 5 | 0.31 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 20 | 0.31 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 15 | 0.3 |
| (4,447) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 1 | 0.3 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 3 | 0.3 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 19 | 0.3 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 12 | 0.3 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 14 | 0.3 |
| (4,426) | 1:53:A:LEU:HD13 | 1:37:A:LEU:HG | 18 | 0.3 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 7 | 0.3 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 10 | 0.3 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 2 | 0.3 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 6 | 0.3 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 11 | 0.3 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 11 | 0.3 |
| (4,322) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 3 | 0.3 |
| (4,319) | 1:26:A:LEU:HD23 | 1:14:A:VAL:HA | 2 | 0.3 |
| (4,307) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 8 | 0.3 |
| (4,307) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 18 | 0.3 |
| (4,299) | 1:168:A:ILE:HD11 | 1:96:A:VAL:HA | 8 | 0.3 |
| (4,208) | 1:171:A:VAL:HG23 | 1:173:A:ALA:HA | 6 | 0.3 |
| (4,195) | 1:114:A:ILE:HD11 | 1:117:A:MET:HE1 | 20 | 0.3 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 10 | 0.3 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB3 | 2 | 0.3 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 3 | 0.3 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 20 | 0.3 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 1 | 0.3 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 15 | 0.3 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 20 | 0.3 |
| (4,4) | 1:65:A:PHE:HD1 | 1:37:A:LEU:HD23 | 10 | 0.3 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 1 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 8 | 0.3 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 2 | 0.3 |
| (2,3836) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 13 | 0.3 |
| (2,3829) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 3 | 0.3 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 9 | 0.3 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 18 | 0.3 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 13 | 0.3 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 16 | 0.3 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 4 | 0.3 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 10 | 0.3 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 19 | 0.3 |
| (2,3804) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG21 | 6 | 0.3 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 1 | 0.3 |
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 8 | 0.3 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 5 | 0.3 |
| (2,3795) | 1:14:A:VAL:HG22 | 1:21:A:LEU:HG | 20 | 0.3 |
| (2,3789) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HB3 | 1 | 0.3 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 6 | 0.3 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 11 | 0.3 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG22 | 16 | 0.3 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 5 | 0.3 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 8 | 0.3 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 15 | 0.3 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 17 | 0.3 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG12 | 19 | 0.3 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD21 | 6 | 0.3 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 18 | 0.3 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 10 | 0.3 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 18 | 0.3 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 19 | 0.3 |
| (2,3677) | 1:15:A:LEU:HD23 | 1:15:A:LEU:HA | 5 | 0.3 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 1 | 0.3 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 9 | 0.3 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 12 | 0.3 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 12 | 0.3 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 14 | 0.3 |
| (2,3514) | 1:143:A:VAL:HG13 | 1:132:A:ARG:HA | 4 | 0.3 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 5 | 0.3 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 17 | 0.3 |
| (2,3490) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HA | 7 | 0.3 |
| (2,3490) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HA | 11 | 0.3 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 13 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 17 | 0.3 |
| (2,3428) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 14 | 0.3 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 17 | 0.3 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 19 | 0.3 |
| (2,3196) | 1:176:A:ILE:HG21 | 1:176:A:ILE:HB | 9 | 0.3 |
| (2,3175) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 1 | 0.3 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 4 | 0.3 |
| (2,3175) | 1:144:A:LEU:HD21 | 1:144:A:LEU:HG | 19 | 0.3 |
| (2,2949) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 5 | 0.3 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 8 | 0.3 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 13 | 0.3 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 20 | 0.3 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG13 | 12 | 0.3 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 3 | 0.3 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 7 | 0.3 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 15 | 0.3 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 10 | 0.3 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 18 | 0.3 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 10 | 0.3 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 15 | 0.3 |
| (2,1900) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 12 | 0.3 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 5 | 0.3 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 7 | 0.3 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 8 | 0.3 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 11 | 0.3 |
| (2,1874) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 4 | 0.3 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 10 | 0.3 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 14 | 0.3 |
| (2,1864) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 15 | 0.3 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 5 | 0.3 |
| (2,1863) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB3 | 14 | 0.3 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 18 | 0.3 |
| (2,1858) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HD11 | 1 | 0.3 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 12 | 0.3 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 14 | 0.3 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 15 | 0.3 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 16 | 0.3 |
| (2,1850) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD21 | 11 | 0.3 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 6 | 0.3 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 18 | 0.3 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 1 | 0.3 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 7 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1839) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HG12 | 9 | 0.3 |
| (2,1838) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 4 | 0.3 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 3 | 0.3 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 1 | 0.3 |
| (2,1832) | 1:53:A:LEU:HD21 | 1:56:A:ILE:HB | 2 | 0.3 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 3 | 0.3 |
| (2,1832) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 15 | 0.3 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 6 | 0.3 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 9 | 0.3 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 11 | 0.3 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 18 | 0.3 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 16 | 0.3 |
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 17 | 0.3 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 16 | 0.3 |
| (2,1796) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD12 | 18 | 0.3 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 17 | 0.3 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 5 | 0.3 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 11 | 0.3 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 13 | 0.3 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 14 | 0.3 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 18 | 0.3 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 6 | 0.3 |
| (2,1709) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 13 | 0.3 |
| (2,1709) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 18 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 3 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 6 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 7 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 10 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 12 | 0.3 |
| (2,1686) | 1:14:A:VAL:HG23 | 1:19:A:PRO:HA | 20 | 0.3 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 7 | 0.3 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 12 | 0.3 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 9 | 0.3 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 7 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 1 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 2 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 4 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 8 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB2 | 1:28:A:ALA:HA | 13 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 14 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 15 | 0.3 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 16 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 19 | 0.3 |
| (2,1573) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 18 | 0.3 |
| (2,1532) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 14 | 0.3 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 6 | 0.3 |
| (2,1459) | 1:108:A:LEU:HD12 | 2:201:A:NAD:H2A | 5 | 0.3 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 14 | 0.3 |
| (2,1405) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 9 | 0.3 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 1 | 0.3 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 12 | 0.3 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 14 | 0.3 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 16 | 0.3 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 17 | 0.3 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 18 | 0.3 |
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 6 | 0.3 |
| (2,1201) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 6 | 0.3 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 3 | 0.3 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 11 | 0.3 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 17 | 0.3 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 19 | 0.3 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 11 | 0.3 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 4 | 0.3 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 1 | 0.3 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 12 | 0.3 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 20 | 0.3 |
| (2,1075) | 1:56:A:ILE:H | 1:58:A:GLU:H | 18 | 0.3 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 4 | 0.3 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 15 | 0.3 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 15 | 0.3 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 6 | 0.3 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 14 | 0.3 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 3 | 0.3 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 1 | 0.3 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 15 | 0.3 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 10 | 0.3 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 7 | 0.3 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 15 | 0.3 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 8 | 0.3 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB2 | 10 | 0.3 |
| (2,438) | 1:55:A:HIS:H | 1:55:A:HIS:HB3 | 18 | 0.3 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 9 | 0.3 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 13 | 0.3 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 16 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 2 | 0.3 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 5 | 0.3 |
| (2,187) | 1:26:A:LEU:HD22 | 1:26:A:LEU:H | 16 | 0.3 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 2 | 0.3 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 2 | 0.3 |
| (2,120) | 1:177:A:LYS:HB3 | 1:178:A:VAL:H | 2 | 0.3 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 7 | 0.3 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 11 | 0.3 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 4 | 0.3 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 7 | 0.3 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 19 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 1 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 2 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 3 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 4 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 6 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 7 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 8 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 9 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 10 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 11 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 14 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 15 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 16 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 18 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 19 | 0.3 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 20 | 0.3 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 17 | 0.3 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 14 | 0.3 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 16 | 0.3 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 7 | 0.3 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 8 | 0.3 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 1 | 0.29 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 19 | 0.29 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 15 | 0.29 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 4 | 0.29 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 8 | 0.29 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 9 | 0.29 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 9 | 0.29 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 1 | 0.29 |
| (4,426) | 1:53:A:LEU:HD13 | 1:37:A:LEU:HG | 10 | 0.29 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 17 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 7 | 0.29 |
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 2 | 0.29 |
| (4,307) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 1 | 0.29 |
| (4,307) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 9 | 0.29 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 3 | 0.29 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 3 | 0.29 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 16 | 0.29 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 14 | 0.29 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB3 | 3 | 0.29 |
| (4,36) | 1:76:A:ALA:H | 1:11:A:LEU:HD23 | 1 | 0.29 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 2 | 0.29 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 16 | 0.29 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 9 | 0.29 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 10 | 0.29 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 14 | 0.29 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 17 | 0.29 |
| (2,3829) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 11 | 0.29 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 10 | 0.29 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 14 | 0.29 |
| (2,3827) | 1:74:A:ILE:HD11 | 1:74:A:ILE:HG12 | 15 | 0.29 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 11 | 0.29 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 5 | 0.29 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 3 | 0.29 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 12 | 0.29 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 13 | 0.29 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 17 | 0.29 |
| (2,3804) | 1:128:A:ILE:HG21 | 1:129:A:THR:HG22 | 2 | 0.29 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 14 | 0.29 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 1 | 0.29 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 4 | 0.29 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 10 | 0.29 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 13 | 0.29 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 16 | 0.29 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG21 | 16 | 0.29 |
| (2,3718) | 1:158:A:PHE:HB3 | 1:168:A:ILE:HG12 | 4 | 0.29 |
| (2,3710) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HA | 13 | 0.29 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 8 | 0.29 |
| (2,3659) | 1:20:A:ALA:HB2 | 1:20:A:ALA:HA | 15 | 0.29 |
| (2,3600) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 20 | 0.29 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 7 | 0.29 |
| (2,3556) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 7 | 0.29 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 10 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3508) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 16 | 0.29 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 1 | 0.29 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 4 | 0.29 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 11 | 0.29 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 3 | 0.29 |
| (2,3484) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 5 | 0.29 |
| (2,3461) | 1:168:A:ILE:HD11 | 1:156:A:PHE:HB2 | 5 | 0.29 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 6 | 0.29 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 8 | 0.29 |
| (2,3434) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HE1 | 3 | 0.29 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 17 | 0.29 |
| (2,3409) | 1:84:A:VAL:HG12 | 1:85:A:ASP:H | 8 | 0.29 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 3 | 0.29 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 17 | 0.29 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 18 | 0.29 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 18 | 0.29 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 19 | 0.29 |
| (2,3355) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 20 | 0.29 |
| (2,3266) | 1:53:A:LEU:HD11 | 1:67:A:PHE:HE1 | 18 | 0.29 |
| (2,3175) | 1:144:A:LEU:HD23 | 1:144:A:LEU:HG | 5 | 0.29 |
| (2,3175) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 11 | 0.29 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 7 | 0.29 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 1 | 0.29 |
| (2,2201) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 20 | 0.29 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 6 | 0.29 |
| (2,2123) | 1:86:A:LEU:H | 1:86:A:LEU:HB3 | 13 | 0.29 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 13 | 0.29 |
| (2,2065) | 1:171:A:VAL:H | 1:168:A:ILE:HG21 | 7 | 0.29 |
| (2,2041) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 1 | 0.29 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 13 | 0.29 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 17 | 0.29 |
| (2,2041) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 19 | 0.29 |
| (2,1974) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 18 | 0.29 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 6 | 0.29 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 1 | 0.29 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 15 | 0.29 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 18 | 0.29 |
| (2,1874) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 11 | 0.29 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 13 | 0.29 |
| (2,1864) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 17 | 0.29 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 15 | 0.29 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 18 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1857) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 2 | 0.29 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 14 | 0.29 |
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD21 | 14 | 0.29 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 10 | 0.29 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 20 | 0.29 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 5 | 0.29 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 10 | 0.29 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 12 | 0.29 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 15 | 0.29 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 7 | 0.29 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 11 | 0.29 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 20 | 0.29 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 1 | 0.29 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 2 | 0.29 |
| (2,1822) | 1:143:A:VAL:HG11 | 1:143:A:VAL:HB | 8 | 0.29 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 14 | 0.29 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 15 | 0.29 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 17 | 0.29 |
| (2,1822) | 1:143:A:VAL:HG11 | 1:143:A:VAL:HB | 20 | 0.29 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 13 | 0.29 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 8 | 0.29 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 17 | 0.29 |
| (2,1796) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD11 | 5 | 0.29 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 6 | 0.29 |
| (2,1796) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD12 | 14 | 0.29 |
| (2,1794) | 1:117:A:MET:HE1 | 1:117:A:MET:HB2 | 6 | 0.29 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 16 | 0.29 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 2 | 0.29 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 18 | 0.29 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 15 | 0.29 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 19 | 0.29 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 2 | 0.29 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 8 | 0.29 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 11 | 0.29 |
| (2,1686) | 1:14:A:VAL:HG23 | 1:19:A:PRO:HA | 13 | 0.29 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 16 | 0.29 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 18 | 0.29 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 11 | 0.29 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 13 | 0.29 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 9 | 0.29 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 11 | 0.29 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 9 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1586) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 10 | 0.29 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 11 | 0.29 |
| (2,1586) | 1:28:A:ALA:HB3 | 1:28:A:ALA:HA | 18 | 0.29 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 20 | 0.29 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 11 | 0.29 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 20 | 0.29 |
| (2,1573) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 6 | 0.29 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 8 | 0.29 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 11 | 0.29 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 14 | 0.29 |
| (2,1514) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 17 | 0.29 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 4 | 0.29 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 9 | 0.29 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 11 | 0.29 |
| (2,1459) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 2 | 0.29 |
| (2,1395) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 10 | 0.29 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 12 | 0.29 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 12 | 0.29 |
| (2,1377) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 2 | 0.29 |
| (2,1301) | 1:34:A:VAL:HG12 | 1:38:A:LEU:H | 4 | 0.29 |
| (2,1201) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 3 | 0.29 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 7 | 0.29 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 8 | 0.29 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 16 | 0.29 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 18 | 0.29 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 3 | 0.29 |
| (2,1193) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 6 | 0.29 |
| (2,1183) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H2N | 2 | 0.29 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 6 | 0.29 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 5 | 0.29 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 16 | 0.29 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 6 | 0.29 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 8 | 0.29 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 18 | 0.29 |
| (2,708) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 3 | 0.29 |
| (2,708) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 7 | 0.29 |
| (2,629) | 1:44:A:LYS:H | 1:42:A:LYS:HG3 | 16 | 0.29 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 10 | 0.29 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 17 | 0.29 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 20 | 0.29 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 10 | 0.29 |
| (2,405) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 17 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 4 | 0.29 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 12 | 0.29 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 3 | 0.29 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 1 | 0.29 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 17 | 0.29 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 18 | 0.29 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 19 | 0.29 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 4 | 0.29 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 18 | 0.29 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 1 | 0.29 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 16 | 0.29 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 17 | 0.29 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 3 | 0.29 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 10 | 0.29 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 13 | 0.29 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 1 | 0.29 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 20 | 0.29 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 12 | 0.29 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 13 | 0.29 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 17 | 0.29 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 3 | 0.29 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 8 | 0.29 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 14 | 0.29 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 1 | 0.29 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 3 | 0.29 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 19 | 0.29 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 14 | 0.29 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 17 | 0.29 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 2 | 0.28 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 13 | 0.28 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 2 | 0.28 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 3 | 0.28 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 5 | 0.28 |
| (4,426) | 1:53:A:LEU:HD13 | 1:37:A:LEU:HG | 6 | 0.28 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 15 | 0.28 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 19 | 0.28 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 20 | 0.28 |
| (4,409) | 1:4:A:MET:HE1 | 1:59:A:THR:HG23 | 20 | 0.28 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 5 | 0.28 |
| (4,395) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HA | 14 | 0.28 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 13 | 0.28 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 18 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,371) | 1:174:A:GLU:HB3 | 1:109:A:ILE:HA | 16 | 0.28 |
| (4,320) | 1:151:A:MET:HE1 | 1:147:A:ASP:HB2 | 18 | 0.28 |
| (4,319) | 1:26:A:LEU:HD23 | 1:14:A:VAL:HA | 10 | 0.28 |
| (4,310) | 1:21:A:LEU:HD13 | 1:10:A:PHE:HA | 12 | 0.28 |
| (4,307) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 6 | 0.28 |
| (4,307) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 15 | 0.28 |
| (4,307) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 17 | 0.28 |
| (4,278) | 1:142:A:VAL:HG13 | 1:102:A:ALA:H | 14 | 0.28 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 7 | 0.28 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 14 | 0.28 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB3 | 12 | 0.28 |
| (4,103) | 1:114:A:ILE:H | 1:144:A:LEU:HA | 1 | 0.28 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 13 | 0.28 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 14 | 0.28 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 17 | 0.28 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 4 | 0.28 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 6 | 0.28 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 13 | 0.28 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 15 | 0.28 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 18 | 0.28 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 19 | 0.28 |
| (2,3836) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 1 | 0.28 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 17 | 0.28 |
| (2,3829) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 1 | 0.28 |
| (2,3827) | 1:74:A:ILE:HD12 | 1:74:A:ILE:HG12 | 17 | 0.28 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 9 | 0.28 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 14 | 0.28 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 6 | 0.28 |
| (2,3821) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 9 | 0.28 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 15 | 0.28 |
| (2,3821) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 18 | 0.28 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 4 | 0.28 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 5 | 0.28 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 7 | 0.28 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 16 | 0.28 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 4 | 0.28 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 8 | 0.28 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD11 | 14 | 0.28 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 6 | 0.28 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 1 | 0.28 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 7 | 0.28 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 10 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 2 | 0.28 |
| (2,3780) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 4 | 0.28 |
| (2,3780) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 7 | 0.28 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 12 | 0.28 |
| (2,3769) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HB | 11 | 0.28 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 3 | 0.28 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG12 | 14 | 0.28 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 4 | 0.28 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 18 | 0.28 |
| (2,3745) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 6 | 0.28 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 4 | 0.28 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 10 | 0.28 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 13 | 0.28 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 14 | 0.28 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 17 | 0.28 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 16 | 0.28 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 20 | 0.28 |
| (2,3559) | 1:102:A:ALA:HB1 | 2:201:A:NAD:H4B | 11 | 0.28 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 13 | 0.28 |
| (2,3514) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 18 | 0.28 |
| (2,3508) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 5 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 2 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 3 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 5 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 10 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 12 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 13 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 14 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 18 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 19 | 0.28 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 20 | 0.28 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 10 | 0.28 |
| (2,3484) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 12 | 0.28 |
| (2,3484) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 20 | 0.28 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 5 | 0.28 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 3 | 0.28 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 15 | 0.28 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 3 | 0.28 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 9 | 0.28 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 16 | 0.28 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 5 | 0.28 |
| (2,3387) | 1:21:A:LEU:HD23 | 1:10:A:PHE:HE1 | 10 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3211) | 1:151:A:MET:HE1 | 1:156:A:PHE:HZ | 17 | 0.28 |
| (2,3182) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 13 | 0.28 |
| (2,3178) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HB2 | 12 | 0.28 |
| (2,3175) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 6 | 0.28 |
| (2,2918) | 1:76:A:ALA:HB1 | 1:78:A:GLN:HE22 | 8 | 0.28 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 14 | 0.28 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 13 | 0.28 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 1 | 0.28 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 1 | 0.28 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 1 | 0.28 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 5 | 0.28 |
| (2,2041) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 8 | 0.28 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 16 | 0.28 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 18 | 0.28 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 8 | 0.28 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 6 | 0.28 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 9 | 0.28 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 10 | 0.28 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 14 | 0.28 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 15 | 0.28 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 17 | 0.28 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 18 | 0.28 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 19 | 0.28 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 1 | 0.28 |
| (2,1863) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB3 | 6 | 0.28 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 4 | 0.28 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 6 | 0.28 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 7 | 0.28 |
| (2,1858) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HD11 | 11 | 0.28 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 16 | 0.28 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 3 | 0.28 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 19 | 0.28 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 10 | 0.28 |
| (2,1841) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 18 | 0.28 |
| (2,1838) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 5 | 0.28 |
| (2,1822) | 1:143:A:VAL:HG11 | 1:143:A:VAL:HB | 4 | 0.28 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 10 | 0.28 |
| (2,1822) | 1:143:A:VAL:HG12 | 1:143:A:VAL:HB | 12 | 0.28 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 16 | 0.28 |
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 11 | 0.28 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 19 | 0.28 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 12 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 7 | 0.28 |
| (2,1737) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 10 | 0.28 |
| (2,1709) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 6 | 0.28 |
| (2,1709) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 8 | 0.28 |
| (2,1709) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 12 | 0.28 |
| (2,1709) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 16 | 0.28 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 1 | 0.28 |
| (2,1686) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 14 | 0.28 |
| (2,1590) | 1:32:A:ALA:HB2 | 1:33:A:PRO:HD3 | 12 | 0.28 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 4 | 0.28 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 10 | 0.28 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 13 | 0.28 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 19 | 0.28 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 12 | 0.28 |
| (2,1492) | 1:167:A:LEU:HD22 | 1:123:A:HIS:HA | 13 | 0.28 |
| (2,1458) | 1:165:A:VAL:HG13 | 2:201:A:NAD:H5N | 7 | 0.28 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 17 | 0.28 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 1 | 0.28 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 1 | 0.28 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 6 | 0.28 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 8 | 0.28 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 6 | 0.28 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 2 | 0.28 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 10 | 0.28 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 13 | 0.28 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 15 | 0.28 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 7 | 0.28 |
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 17 | 0.28 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD11 | 14 | 0.28 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 15 | 0.28 |
| (2,1211) | 1:177:A:LYS:HD2 | 1:177:A:LYS:HA | 16 | 0.28 |
| (2,1200) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 9 | 0.28 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 17 | 0.28 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 4 | 0.28 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 5 | 0.28 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 19 | 0.28 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 8 | 0.28 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 11 | 0.28 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 12 | 0.28 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 14 | 0.28 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 18 | 0.28 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 15 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 6 | 0.28 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 10 | 0.28 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 5 | 0.28 |
| (2,383) | 1:20:A:ALA:H | 1:19:A:PRO:HD3 | 1 | 0.28 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 15 | 0.28 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 3 | 0.28 |
| (2,232) | 1:109:A:ILE:H | 1:102:A:ALA:H | 20 | 0.28 |
| (2,202) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 1 | 0.28 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 4 | 0.28 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 6 | 0.28 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 8 | 0.28 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 10 | 0.28 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 12 | 0.28 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 13 | 0.28 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 14 | 0.28 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 16 | 0.28 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 3 | 0.28 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 20 | 0.28 |
| (2,164) | 1:86:A:LEU:H | 1:86:A:LEU:HB3 | 13 | 0.28 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 2 | 0.28 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 3 | 0.28 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 20 | 0.28 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 5 | 0.28 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 1 | 0.28 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 12 | 0.28 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 16 | 0.28 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 20 | 0.28 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 18 | 0.28 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 8 | 0.28 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 20 | 0.28 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 5 | 0.28 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 9 | 0.28 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 13 | 0.28 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 1 | 0.28 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 3 | 0.28 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 8 | 0.28 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 12 | 0.28 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 2 | 0.28 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 4 | 0.28 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 6 | 0.28 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 9 | 0.28 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 10 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 11 | 0.28 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 18 | 0.28 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 14 | 0.28 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 8 | 0.27 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 9 | 0.27 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 17 | 0.27 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 16 | 0.27 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 7 | 0.27 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 17 | 0.27 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 14 | 0.27 |
| (4,436) | 1:34:A:VAL:HG11 | 1:35:A:LYS:HG3 | 18 | 0.27 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 4 | 0.27 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 7 | 0.27 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 9 | 0.27 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 11 | 0.27 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 13 | 0.27 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 16 | 0.27 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 6 | 0.27 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 18 | 0.27 |
| (4,307) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 7 | 0.27 |
| (4,307) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 10 | 0.27 |
| (4,307) | 1:38:A:LEU:HD12 | 1:50:A:MET:HA | 11 | 0.27 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 18 | 0.27 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 4 | 0.27 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 19 | 0.27 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 1 | 0.27 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 6 | 0.27 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 20 | 0.27 |
| (2,3832) | 1:97:A:LEU:HD22 | 1:151:A:MET:HG3 | 5 | 0.27 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 4 | 0.27 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 6 | 0.27 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 16 | 0.27 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG22 | 5 | 0.27 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 14 | 0.27 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 17 | 0.27 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 9 | 0.27 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 7 | 0.27 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 10 | 0.27 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 13 | 0.27 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 10 | 0.27 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 4 | 0.27 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 20 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3763) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD12 | 16 | 0.27 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 1 | 0.27 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG11 | 11 | 0.27 |
| (2,3748) | 1:108:A:LEU:HG | 1:108:A:LEU:HD23 | 19 | 0.27 |
| (2,3718) | 1:158:A:PHE:HB2 | 1:168:A:ILE:HG12 | 17 | 0.27 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 7 | 0.27 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 9 | 0.27 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 16 | 0.27 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 6 | 0.27 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 7 | 0.27 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 8 | 0.27 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 9 | 0.27 |
| (2,3496) | 1:38:A:LEU:HD23 | 1:38:A:LEU:HA | 15 | 0.27 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 12 | 0.27 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 8 | 0.27 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 9 | 0.27 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 13 | 0.27 |
| (2,3479) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 18 | 0.27 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 3 | 0.27 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 18 | 0.27 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 20 | 0.27 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 8 | 0.27 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 11 | 0.27 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 14 | 0.27 |
| (2,3404) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 6 | 0.27 |
| (2,3399) | 1:21:A:LEU:HD13 | 1:21:A:LEU:H | 20 | 0.27 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 4 | 0.27 |
| (2,3346) | 1:4:A:MET:HE3 | 1:55:A:HIS:HD2 | 2 | 0.27 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 8 | 0.27 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 10 | 0.27 |
| (2,3175) | 1:144:A:LEU:HD22 | 1:144:A:LEU:HG | 3 | 0.27 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 1 | 0.27 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 4 | 0.27 |
| (2,2308) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 2 | 0.27 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 13 | 0.27 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 12 | 0.27 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 12 | 0.27 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 3 | 0.27 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 19 | 0.27 |
| (2,1936) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 12 | 0.27 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 1 | 0.27 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 4 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 13 | 0.27 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 19 | 0.27 |
| (2,1874) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 7 | 0.27 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 3 | 0.27 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 4 | 0.27 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 13 | 0.27 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 16 | 0.27 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD11 | 6 | 0.27 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 3 | 0.27 |
| (2,1858) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HD11 | 5 | 0.27 |
| (2,1858) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 13 | 0.27 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 12 | 0.27 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 10 | 0.27 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 17 | 0.27 |
| (2,1844) | 1:110:A:LEU:HD23 | 1:110:A:LEU:HB3 | 9 | 0.27 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 8 | 0.27 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 1 | 0.27 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 3 | 0.27 |
| (2,1822) | 1:143:A:VAL:HG13 | 1:143:A:VAL:HB | 19 | 0.27 |
| (2,1817) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 4 | 0.27 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 4 | 0.27 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 10 | 0.27 |
| (2,1796) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD11 | 15 | 0.27 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 7 | 0.27 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 16 | 0.27 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 15 | 0.27 |
| (2,1709) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 14 | 0.27 |
| (2,1686) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 17 | 0.27 |
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 16 | 0.27 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 3 | 0.27 |
| (2,1599) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 8 | 0.27 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 3 | 0.27 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 11 | 0.27 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 2 | 0.27 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 3 | 0.27 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 15 | 0.27 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 20 | 0.27 |
| (2,1586) | 1:28:A:ALA:HB1 | 1:28:A:ALA:HA | 7 | 0.27 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 1 | 0.27 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 2 | 0.27 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 4 | 0.27 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 7 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 13 | 0.27 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 15 | 0.27 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 20 | 0.27 |
| (2,1563) | 1:48:A:ILE:HG23 | 1:53:A:LEU:HB2 | 2 | 0.27 |
| (2,1555) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 6 | 0.27 |
| (2,1535) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HE3 | 17 | 0.27 |
| (2,1514) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 5 | 0.27 |
| (2,1461) | 1:128:A:ILE:HD13 | 1:127:A:ASP:H | 14 | 0.27 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 3 | 0.27 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 9 | 0.27 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 16 | 0.27 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 9 | 0.27 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 12 | 0.27 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 15 | 0.27 |
| (2,1426) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HD1 | 1 | 0.27 |
| (2,1420) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HE1 | 4 | 0.27 |
| (2,1420) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HE1 | 15 | 0.27 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 16 | 0.27 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 10 | 0.27 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 15 | 0.27 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 17 | 0.27 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 19 | 0.27 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 9 | 0.27 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 8 | 0.27 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 9 | 0.27 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 11 | 0.27 |
| (2,1301) | 1:34:A:VAL:HG12 | 1:38:A:LEU:H | 6 | 0.27 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 9 | 0.27 |
| (2,1301) | 1:34:A:VAL:HG12 | 1:38:A:LEU:H | 11 | 0.27 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 10 | 0.27 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 2 | 0.27 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD11 | 5 | 0.27 |
| (2,1187) | 1:176:A:ILE:HG21 | 1:106:A:PHE:HE1 | 12 | 0.27 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 14 | 0.27 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 5 | 0.27 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 18 | 0.27 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 16 | 0.27 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 20 | 0.27 |
| (2,815) | 1:102:A:ALA:H | 1:101:A:THR:HG23 | 20 | 0.27 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD13 | 5 | 0.27 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD13 | 6 | 0.27 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD12 | 13 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 18 | 0.27 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 10 | 0.27 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 17 | 0.27 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 19 | 0.27 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 14 | 0.27 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 1 | 0.27 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 18 | 0.27 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 16 | 0.27 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD12 | 10 | 0.27 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 12 | 0.27 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 5 | 0.27 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 5 | 0.27 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 19 | 0.27 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 2 | 0.27 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 5 | 0.27 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 7 | 0.27 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 9 | 0.27 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 15 | 0.27 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 20 | 0.27 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 15 | 0.27 |
| (2,120) | 1:177:A:LYS:HB3 | 1:178:A:VAL:H | 11 | 0.27 |
| (2,33) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HZ | 5 | 0.27 |
| (2,16) | 1:21:A:LEU:HD13 | 1:10:A:PHE:HE1 | 3 | 0.27 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 7 | 0.27 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 9 | 0.27 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 19 | 0.27 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 3 | 0.27 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 13 | 0.27 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 16 | 0.27 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 5 | 0.27 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 1 | 0.27 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 1 | 0.27 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 10 | 0.27 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 17 | 0.27 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 13 | 0.27 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 13 | 0.27 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 15 | 0.27 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 16 | 0.27 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 18 | 0.26 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD11 | 9 | 0.26 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 8 | 0.26 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 17 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 12 | 0.26 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 8 | 0.26 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 14 | 0.26 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 4 | 0.26 |
| (4,307) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 16 | 0.26 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 1 | 0.26 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 9 | 0.26 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 12 | 0.26 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB3 | 1 | 0.26 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB3 | 8 | 0.26 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 5 | 0.26 |
| (4,40) | 1:5:A:VAL:H | 1:5:A:VAL:HB | 10 | 0.26 |
| (4,40) | 1:5:A:VAL:H | 1:5:A:VAL:HB | 11 | 0.26 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 3 | 0.26 |
| (2,3964) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H6N | 8 | 0.26 |
| (2,3959) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H5N | 1 | 0.26 |
| (2,3844) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 2 | 0.26 |
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 20 | 0.26 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 3 | 0.26 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 7 | 0.26 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD11 | 6 | 0.26 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 17 | 0.26 |
| (2,3821) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 2 | 0.26 |
| (2,3821) | 1:144:A:LEU:HD13 | 1:109:A:ILE:HG21 | 4 | 0.26 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 11 | 0.26 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 17 | 0.26 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 2 | 0.26 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 3 | 0.26 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 5 | 0.26 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 6 | 0.26 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 13 | 0.26 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 16 | 0.26 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 16 | 0.26 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 2 | 0.26 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 15 | 0.26 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 17 | 0.26 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 18 | 0.26 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD11 | 19 | 0.26 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 3 | 0.26 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 6 | 0.26 |
| (2,3769) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HB | 10 | 0.26 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 13 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 19 | 0.26 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 4 | 0.26 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 1 | 0.26 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD22 | 2 | 0.26 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD22 | 3 | 0.26 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 12 | 0.26 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 15 | 0.26 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 18 | 0.26 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE2 | 15 | 0.26 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 6 | 0.26 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 14 | 0.26 |
| (2,3490) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HA | 5 | 0.26 |
| (2,3490) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HA | 16 | 0.26 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 17 | 0.26 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 12 | 0.26 |
| (2,3409) | 1:84:A:VAL:HG11 | 1:85:A:ASP:H | 9 | 0.26 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 15 | 0.26 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 18 | 0.26 |
| (2,3288) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 3 | 0.26 |
| (2,3182) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 17 | 0.26 |
| (2,2738) | 1:30:A:GLY:H | 1:26:A:LEU:HD23 | 16 | 0.26 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 16 | 0.26 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 18 | 0.26 |
| (2,2148) | 1:26:A:LEU:HD23 | 1:26:A:LEU:H | 19 | 0.26 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 17 | 0.26 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 1 | 0.26 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 10 | 0.26 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 3 | 0.26 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 6 | 0.26 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 7 | 0.26 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 10 | 0.26 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 11 | 0.26 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 15 | 0.26 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 20 | 0.26 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 4 | 0.26 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 8 | 0.26 |
| (2,1869) | 1:97:A:LEU:HD23 | 1:96:A:VAL:HB | 6 | 0.26 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 11 | 0.26 |
| (2,1857) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 4 | 0.26 |
| (2,1857) | 1:151:A:MET:HE2 | 1:171:A:VAL:HG12 | 7 | 0.26 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 3 | 0.26 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 20 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1850) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 2 | 0.26 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 3 | 0.26 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 2 | 0.26 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD11 | 4 | 0.26 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 11 | 0.26 |
| (2,1844) | 1:110:A:LEU:HD23 | 1:110:A:LEU:HB3 | 12 | 0.26 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 14 | 0.26 |
| (2,1844) | 1:110:A:LEU:HD23 | 1:110:A:LEU:HB3 | 16 | 0.26 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 11 | 0.26 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 18 | 0.26 |
| (2,1807) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 17 | 0.26 |
| (2,1796) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD11 | 1 | 0.26 |
| (2,1796) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD12 | 13 | 0.26 |
| (2,1796) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD11 | 17 | 0.26 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 6 | 0.26 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 14 | 0.26 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 12 | 0.26 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 15 | 0.26 |
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 5 | 0.26 |
| (2,1640) | 1:40:A:LYS:HE3 | 1:25:A:ASP:HB2 | 9 | 0.26 |
| (2,1633) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 3 | 0.26 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 16 | 0.26 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE1 | 7 | 0.26 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 1 | 0.26 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 8 | 0.26 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 12 | 0.26 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 14 | 0.26 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 16 | 0.26 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 17 | 0.26 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 6 | 0.26 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 9 | 0.26 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 12 | 0.26 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 14 | 0.26 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 15 | 0.26 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 18 | 0.26 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 19 | 0.26 |
| (2,1573) | 1:66:A:ALA:HB1 | 1:66:A:ALA:HA | 3 | 0.26 |
| (2,1514) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 12 | 0.26 |
| (2,1514) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 20 | 0.26 |
| (2,1492) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 17 | 0.26 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 11 | 0.26 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1435) | 1:15:A:LEU:HD23 | 1:15:A:LEU:H | 12 | 0.26 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 18 | 0.26 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 6 | 0.26 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 8 | 0.26 |
| (2,1378) | 1:50:A:MET:HE3 | 1:67:A:PHE:HZ | 3 | 0.26 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 18 | 0.26 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 7 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 1 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 3 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 4 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 7 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 14 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 16 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 18 | 0.26 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 19 | 0.26 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 9 | 0.26 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 10 | 0.26 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB3 | 20 | 0.26 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 4 | 0.26 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 10 | 0.26 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 16 | 0.26 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 2 | 0.26 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 2 | 0.26 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 13 | 0.26 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 15 | 0.26 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 19 | 0.26 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 10 | 0.26 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 19 | 0.26 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 4 | 0.26 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 5 | 0.26 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 17 | 0.26 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 7 | 0.26 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 9 | 0.26 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 12 | 0.26 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 15 | 0.26 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 12 | 0.26 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD13 | 8 | 0.26 |
| (2,768) | 1:30:A:GLY:H | 1:26:A:LEU:HD21 | 3 | 0.26 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 9 | 0.26 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 16 | 0.26 |
| (2,726) | 1:20:A:ALA:HB2 | 1:23:A:GLY:H | 3 | 0.26 |
| (2,708) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 4 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,708) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 19 | 0.26 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 14 | 0.26 |
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 11 | 0.26 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 2 | 0.26 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 3 | 0.26 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 5 | 0.26 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 19 | 0.26 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 14 | 0.26 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 12 | 0.26 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 5 | 0.26 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 11 | 0.26 |
| (2,289) | 1:46:A:HIS:H | 1:22:A:ILE:HG22 | 20 | 0.26 |
| (2,206) | 1:76:A:ALA:H | 1:15:A:LEU:HD11 | 9 | 0.26 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 1 | 0.26 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 11 | 0.26 |
| (2,145) | 1:83:A:GLU:HB3 | 1:83:A:GLU:H | 7 | 0.26 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 4 | 0.26 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 6 | 0.26 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 11 | 0.26 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 12 | 0.26 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 11 | 0.26 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 13 | 0.26 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 1 | 0.26 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 8 | 0.26 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 9 | 0.26 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 13 | 0.26 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 20 | 0.26 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 6 | 0.26 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 12 | 0.26 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 12 | 0.26 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 13 | 0.26 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 20 | 0.26 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 12 | 0.26 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 15 | 0.26 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 12 | 0.26 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 7 | 0.26 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 20 | 0.26 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 7 | 0.26 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 6 | 0.26 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 1 | 0.26 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 17 | 0.26 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 3 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,452) | 1:59:A:THR:HB | 1:59:A:THR:HG22 | 13 | 0.25 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 13 | 0.25 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 17 | 0.25 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 19 | 0.25 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 20 | 0.25 |
| (4,443) | 1:48:A:ILE:HD12 | 1:38:A:LEU:HB2 | 14 | 0.25 |
| (4,426) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 17 | 0.25 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 2 | 0.25 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 13 | 0.25 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 15 | 0.25 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 12 | 0.25 |
| (4,364) | 1:4:A:MET:HE2 | 1:53:A:LEU:HB2 | 18 | 0.25 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 7 | 0.25 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 6 | 0.25 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 11 | 0.25 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 4 | 0.25 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 5 | 0.25 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 14 | 0.25 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 12 | 0.25 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 8 | 0.25 |
| (2,3832) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 20 | 0.25 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 19 | 0.25 |
| (2,3824) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 17 | 0.25 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 1 | 0.25 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 5 | 0.25 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 11 | 0.25 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 12 | 0.25 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 15 | 0.25 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 20 | 0.25 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 3 | 0.25 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 11 | 0.25 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 13 | 0.25 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 7 | 0.25 |
| (2,3809) | 1:110:A:LEU:HD13 | 1:176:A:ILE:HB | 15 | 0.25 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 20 | 0.25 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 4 | 0.25 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 8 | 0.25 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 9 | 0.25 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 17 | 0.25 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 19 | 0.25 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 20 | 0.25 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 19 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 4 | 0.25 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 11 | 0.25 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 6 | 0.25 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 9 | 0.25 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 19 | 0.25 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 17 | 0.25 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 4 | 0.25 |
| (2,3772) | 1:151:A:MET:HE3 | 1:174:A:GLU:HG2 | 5 | 0.25 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 10 | 0.25 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 3 | 0.25 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 4 | 0.25 |
| (2,3769) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HB | 5 | 0.25 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 16 | 0.25 |
| (2,3769) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 17 | 0.25 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 9 | 0.25 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 17 | 0.25 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 17 | 0.25 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 10 | 0.25 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 1 | 0.25 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 6 | 0.25 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 8 | 0.25 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 9 | 0.25 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 11 | 0.25 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 18 | 0.25 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 6 | 0.25 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 11 | 0.25 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 12 | 0.25 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE1 | 7 | 0.25 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 9 | 0.25 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 13 | 0.25 |
| (2,3439) | 1:110:A:LEU:HD11 | 1:110:A:LEU:H | 14 | 0.25 |
| (2,3434) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HE1 | 19 | 0.25 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 6 | 0.25 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 8 | 0.25 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 9 | 0.25 |
| (2,2625) | 1:29:A:ASN:H | 1:29:A:ASN:HB3 | 9 | 0.25 |
| (2,2625) | 1:29:A:ASN:H | 1:29:A:ASN:HB3 | 18 | 0.25 |
| (2,2575) | 1:111:A:LYS:HB2 | 1:111:A:LYS:H | 8 | 0.25 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 13 | 0.25 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 10 | 0.25 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 14 | 0.25 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG11 | 18 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 11 | 0.25 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 18 | 0.25 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 15 | 0.25 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 19 | 0.25 |
| (2,2123) | 1:86:A:LEU:H | 1:86:A:LEU:HB3 | 20 | 0.25 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 13 | 0.25 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 18 | 0.25 |
| (2,2041) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 2 | 0.25 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 2 | 0.25 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 15 | 0.25 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 11 | 0.25 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 17 | 0.25 |
| (2,1889) | 1:4:A:MET:HE1 | 1:4:A:MET:HA | 3 | 0.25 |
| (2,1881) | 1:24:A:LEU:HD11 | 1:33:A:PRO:HD3 | 2 | 0.25 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 13 | 0.25 |
| (2,1869) | 1:97:A:LEU:HD21 | 1:96:A:VAL:HB | 18 | 0.25 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 19 | 0.25 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 4 | 0.25 |
| (2,1861) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 17 | 0.25 |
| (2,1857) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 5 | 0.25 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 19 | 0.25 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 1 | 0.25 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG22 | 13 | 0.25 |
| (2,1854) | 1:22:A:ILE:HG23 | 1:14:A:VAL:HG21 | 16 | 0.25 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 14 | 0.25 |
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 8 | 0.25 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 2 | 0.25 |
| (2,1844) | 1:110:A:LEU:HD22 | 1:110:A:LEU:HB3 | 6 | 0.25 |
| (2,1844) | 1:110:A:LEU:HD23 | 1:110:A:LEU:HB3 | 13 | 0.25 |
| (2,1844) | 1:110:A:LEU:HD22 | 1:110:A:LEU:HB3 | 15 | 0.25 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 5 | 0.25 |
| (2,1815) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HB2 | 10 | 0.25 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 6 | 0.25 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 9 | 0.25 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 12 | 0.25 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 15 | 0.25 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 8 | 0.25 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 3 | 0.25 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 11 | 0.25 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 15 | 0.25 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 1 | 0.25 |
| (2,1709) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1709) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 7 | 0.25 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 4 | 0.25 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 5 | 0.25 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 19 | 0.25 |
| (2,1587) | 1:11:A:LEU:HG | 1:11:A:LEU:HA | 5 | 0.25 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 5 | 0.25 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 8 | 0.25 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 10 | 0.25 |
| (2,1573) | 1:66:A:ALA:HB3 | 1:66:A:ALA:HA | 5 | 0.25 |
| (2,1524) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 13 | 0.25 |
| (2,1509) | 1:151:A:MET:HE3 | 1:171:A:VAL:HA | 20 | 0.25 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 8 | 0.25 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 14 | 0.25 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 15 | 0.25 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 10 | 0.25 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 3 | 0.25 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 16 | 0.25 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 1 | 0.25 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 2 | 0.25 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 4 | 0.25 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 10 | 0.25 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 11 | 0.25 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 15 | 0.25 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 18 | 0.25 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 11 | 0.25 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 5 | 0.25 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 6 | 0.25 |
| (2,1301) | 1:34:A:VAL:HG13 | 1:38:A:LEU:H | 1 | 0.25 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 2 | 0.25 |
| (2,1288) | 1:167:A:LEU:HD22 | 1:167:A:LEU:HA | 1 | 0.25 |
| (2,1288) | 1:167:A:LEU:HD22 | 1:167:A:LEU:HA | 20 | 0.25 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 8 | 0.25 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 11 | 0.25 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 12 | 0.25 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 15 | 0.25 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 19 | 0.25 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 15 | 0.25 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 2 | 0.25 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 3 | 0.25 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 6 | 0.25 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 7 | 0.25 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 11 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 12 | 0.25 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 15 | 0.25 |
| (2,1194) | 1:176:A:ILE:HD12 | 1:114:A:ILE:HD13 | 6 | 0.25 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 16 | 0.25 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 1 | 0.25 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 3 | 0.25 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 10 | 0.25 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 12 | 0.25 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 13 | 0.25 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 15 | 0.25 |
| (2,1131) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 2 | 0.25 |
| (2,1131) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 3 | 0.25 |
| (2,1075) | 1:56:A:ILE:H | 1:58:A:GLU:H | 10 | 0.25 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 7 | 0.25 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 8 | 0.25 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 9 | 0.25 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 1 | 0.25 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 3 | 0.25 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 6 | 0.25 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 20 | 0.25 |
| (2,985) | 1:46:A:HIS:H | 1:45:A:GLY:H | 12 | 0.25 |
| (2,985) | 1:46:A:HIS:H | 1:45:A:GLY:H | 14 | 0.25 |
| (2,752) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 20 | 0.25 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 16 | 0.25 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 5 | 0.25 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 20 | 0.25 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 3 | 0.25 |
| (2,550) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 9 | 0.25 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 8 | 0.25 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 11 | 0.25 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 13 | 0.25 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 14 | 0.25 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 19 | 0.25 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 20 | 0.25 |
| (2,486) | 1:58:A:GLU:H | 1:58:A:GLU:HB3 | 15 | 0.25 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 8 | 0.25 |
| (2,201) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 3 | 0.25 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 18 | 0.25 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 1 | 0.25 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 6 | 0.25 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 15 | 0.25 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 16 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 4 | 0.25 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 14 | 0.25 |
| (2,120) | 1:177:A:LYS:HB3 | 1:178:A:VAL:H | 9 | 0.25 |
| (2,120) | 1:177:A:LYS:HB3 | 1:178:A:VAL:H | 16 | 0.25 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 17 | 0.25 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 4 | 0.25 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 6 | 0.25 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 5 | 0.25 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 19 | 0.25 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 5 | 0.25 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 15 | 0.25 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 17 | 0.25 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 18 | 0.25 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 19 | 0.25 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 9 | 0.25 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 10 | 0.25 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 1 | 0.25 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 17 | 0.25 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 20 | 0.25 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 2 | 0.25 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 4 | 0.25 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 12 | 0.25 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 18 | 0.25 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 12 | 0.25 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 4 | 0.25 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 7 | 0.25 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 11 | 0.25 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 14 | 0.25 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 4 | 0.25 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 1 | 0.25 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 3 | 0.25 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 16 | 0.25 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 1 | 0.25 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 4 | 0.25 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 18 | 0.25 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 5 | 0.25 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 12 | 0.25 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 19 | 0.25 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 7 | 0.25 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 9 | 0.25 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 11 | 0.25 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 12 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,452) | 1:59:A:THR:HB | 1:59:A:THR:HG22 | 5 | 0.24 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 7 | 0.24 |
| (4,445) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 12 | 0.24 |
| (4,442) | 1:178:A:VAL:HG22 | 1:176:A:ILE:HB | 17 | 0.24 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 4 | 0.24 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 15 | 0.24 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 20 | 0.24 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 6 | 0.24 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 20 | 0.24 |
| (4,325) | 1:7:A:VAL:HG13 | 1:10:A:PHE:HB3 | 15 | 0.24 |
| (4,319) | 1:26:A:LEU:HD23 | 1:14:A:VAL:HA | 15 | 0.24 |
| (4,311) | 1:143:A:VAL:HG11 | 1:178:A:VAL:HA | 4 | 0.24 |
| (4,307) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 2 | 0.24 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 12 | 0.24 |
| (4,208) | 1:14:A:VAL:HG21 | 1:11:A:LEU:HA | 13 | 0.24 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB3 | 14 | 0.24 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 2 | 0.24 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 13 | 0.24 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 9 | 0.24 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 10 | 0.24 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 19 | 0.24 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD21 | 20 | 0.24 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD22 | 5 | 0.24 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 19 | 0.24 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 14 | 0.24 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 7 | 0.24 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 11 | 0.24 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 20 | 0.24 |
| (2,3841) | 1:76:A:ALA:HB3 | 1:76:A:ALA:H | 15 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 3 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 4 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 9 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 14 | 0.24 |
| (2,3836) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 18 | 0.24 |
| (2,3823) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 8 | 0.24 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 19 | 0.24 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG22 | 10 | 0.24 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 6 | 0.24 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 10 | 0.24 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 8 | 0.24 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 9 | 0.24 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 12 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 15 | 0.24 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 14 | 0.24 |
| (2,3810) | 1:171:A:VAL:HG21 | 1:168:A:ILE:HD13 | 20 | 0.24 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 11 | 0.24 |
| (2,3809) | 1:176:A:ILE:HB | 1:110:A:LEU:HD11 | 14 | 0.24 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 7 | 0.24 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 11 | 0.24 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 14 | 0.24 |
| (2,3800) | 1:56:A:ILE:HD11 | 1:56:A:ILE:HG12 | 6 | 0.24 |
| (2,3800) | 1:56:A:ILE:HD11 | 1:56:A:ILE:HG12 | 7 | 0.24 |
| (2,3800) | 1:56:A:ILE:HD11 | 1:56:A:ILE:HG12 | 9 | 0.24 |
| (2,3800) | 1:56:A:ILE:HD11 | 1:56:A:ILE:HG12 | 17 | 0.24 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 20 | 0.24 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 7 | 0.24 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 8 | 0.24 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 16 | 0.24 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 4 | 0.24 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 7 | 0.24 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 8 | 0.24 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 12 | 0.24 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 16 | 0.24 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 2 | 0.24 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 18 | 0.24 |
| (2,3756) | 1:144:A:LEU:HG | 1:178:A:VAL:HG12 | 7 | 0.24 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 6 | 0.24 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 11 | 0.24 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 12 | 0.24 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 2 | 0.24 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 3 | 0.24 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 15 | 0.24 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD23 | 8 | 0.24 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 20 | 0.24 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 7 | 0.24 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 14 | 0.24 |
| (2,3683) | 1:84:A:VAL:HA | 1:84:A:VAL:HG22 | 1 | 0.24 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 5 | 0.24 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 9 | 0.24 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE2 | 16 | 0.24 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE3 | 19 | 0.24 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 3 | 0.24 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 9 | 0.24 |
| (2,3508) | 1:21:A:LEU:HD12 | 1:44:A:LYS:HE2 | 7 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 12 | 0.24 |
| (2,3495) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 13 | 0.24 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 15 | 0.24 |
| (2,3490) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HA | 19 | 0.24 |
| (2,3479) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 6 | 0.24 |
| (2,3434) | 1:15:A:LEU:HD12 | 1:65:A:PHE:HE1 | 5 | 0.24 |
| (2,3434) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HE1 | 7 | 0.24 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 10 | 0.24 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 12 | 0.24 |
| (2,3409) | 1:84:A:VAL:HG11 | 1:85:A:ASP:H | 12 | 0.24 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 1 | 0.24 |
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 5 | 0.24 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 5 | 0.24 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 5 | 0.24 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 8 | 0.24 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 3 | 0.24 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 15 | 0.24 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 2 | 0.24 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 17 | 0.24 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 3 | 0.24 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 8 | 0.24 |
| (2,2785) | 1:53:A:LEU:H | 1:38:A:LEU:HD11 | 1 | 0.24 |
| (2,2625) | 1:29:A:ASN:H | 1:29:A:ASN:HB3 | 1 | 0.24 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 5 | 0.24 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 5 | 0.24 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 6 | 0.24 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 15 | 0.24 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 19 | 0.24 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 9 | 0.24 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 13 | 0.24 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 16 | 0.24 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 1 | 0.24 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 5 | 0.24 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 20 | 0.24 |
| (2,2266) | 1:153:A:ASP:H | 1:95:A:ALA:HB1 | 11 | 0.24 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 7 | 0.24 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 4 | 0.24 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 2 | 0.24 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 5 | 0.24 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 5 | 0.24 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 7 | 0.24 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 8 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 11 | 0.24 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 12 | 0.24 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 14 | 0.24 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 10 | 0.24 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 16 | 0.24 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD13 | 6 | 0.24 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 7 | 0.24 |
| (2,1857) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 1 | 0.24 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 20 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 7 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 8 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 9 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 10 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 12 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 17 | 0.24 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 19 | 0.24 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 1 | 0.24 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 8 | 0.24 |
| (2,1831) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 12 | 0.24 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 2 | 0.24 |
| (2,1818) | 1:86:A:LEU:HD12 | 1:86:A:LEU:HG | 4 | 0.24 |
| (2,1818) | 1:86:A:LEU:HD13 | 1:86:A:LEU:HG | 7 | 0.24 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 2 | 0.24 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 7 | 0.24 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 13 | 0.24 |
| (2,1804) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HB | 11 | 0.24 |
| (2,1796) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD11 | 7 | 0.24 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 11 | 0.24 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 8 | 0.24 |
| (2,1754) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 14 | 0.24 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 20 | 0.24 |
| (2,1709) | 1:86:A:LEU:HD23 | 1:86:A:LEU:HA | 19 | 0.24 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE2 | 14 | 0.24 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 6 | 0.24 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 8 | 0.24 |
| (2,1576) | 1:22:A:ILE:HG21 | 1:22:A:ILE:HA | 16 | 0.24 |
| (2,1565) | 1:22:A:ILE:HG23 | 1:41:A:MET:HB2 | 3 | 0.24 |
| (2,1534) | 1:151:A:MET:HE3 | 1:151:A:MET:HA | 7 | 0.24 |
| (2,1524) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 17 | 0.24 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 18 | 0.24 |
| (2,1459) | 1:108:A:LEU:HD13 | 2:201:A:NAD:H2A | 18 | 0.24 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 6 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 1 | 0.24 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 2 | 0.24 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 9 | 0.24 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 4 | 0.24 |
| (2,1377) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 5 | 0.24 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 13 | 0.24 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 1 | 0.24 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 12 | 0.24 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 17 | 0.24 |
| (2,1301) | 1:34:A:VAL:HG12 | 1:38:A:LEU:H | 17 | 0.24 |
| (2,1288) | 1:167:A:LEU:HD23 | 1:167:A:LEU:HA | 3 | 0.24 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 3 | 0.24 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 4 | 0.24 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 13 | 0.24 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 16 | 0.24 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 17 | 0.24 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 18 | 0.24 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 1 | 0.24 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 5 | 0.24 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 8 | 0.24 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 13 | 0.24 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 17 | 0.24 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 19 | 0.24 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 20 | 0.24 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 7 | 0.24 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 19 | 0.24 |
| (2,1155) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 17 | 0.24 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 4 | 0.24 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 10 | 0.24 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 16 | 0.24 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 13 | 0.24 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 8 | 0.24 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 12 | 0.24 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 10 | 0.24 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 19 | 0.24 |
| (2,985) | 1:46:A:HIS:H | 1:45:A:GLY:H | 16 | 0.24 |
| (2,985) | 1:46:A:HIS:H | 1:45:A:GLY:H | 17 | 0.24 |
| (2,811) | 1:14:A:VAL:HG21 | 1:22:A:ILE:H | 5 | 0.24 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD11 | 12 | 0.24 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 4 | 0.24 |
| (2,653) | 1:29:A:ASN:H | 1:29:A:ASN:HB3 | 9 | 0.24 |
| (2,653) | 1:29:A:ASN:H | 1:29:A:ASN:HB3 | 18 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,550) | 1:105:A:ASN:H | 1:102:A:ALA:HB3 | 8 | 0.24 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 7 | 0.24 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 2 | 0.24 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 7 | 0.24 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 9 | 0.24 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 17 | 0.24 |
| (2,486) | 1:58:A:GLU:H | 1:58:A:GLU:HB3 | 17 | 0.24 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 12 | 0.24 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 15 | 0.24 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 19 | 0.24 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 6 | 0.24 |
| (2,412) | 1:11:A:LEU:HD11 | 1:11:A:LEU:H | 10 | 0.24 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 11 | 0.24 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 19 | 0.24 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 20 | 0.24 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 3 | 0.24 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 11 | 0.24 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 7 | 0.24 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 19 | 0.24 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 5 | 0.24 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 1 | 0.24 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 7 | 0.24 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 9 | 0.24 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD11 | 4 | 0.24 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD11 | 19 | 0.24 |
| (2,120) | 1:177:A:LYS:HB3 | 1:178:A:VAL:H | 7 | 0.24 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 8 | 0.24 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 18 | 0.24 |
| (2,21) | 1:88:A:TYR:HE1 | 1:86:A:LEU:HD13 | 11 | 0.24 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 2 | 0.24 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 4 | 0.24 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 1 | 0.24 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 2 | 0.24 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 10 | 0.24 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 5 | 0.24 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 1 | 0.24 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 7 | 0.24 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 8 | 0.24 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 2 | 0.24 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 4 | 0.24 |
| (1,84) | 1:122:A:VAL:N | 1:168:A:ILE:O | 17 | 0.24 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 3 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 16 | 0.24 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 8 | 0.24 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 15 | 0.24 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 6 | 0.24 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 15 | 0.24 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 4 | 0.24 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 19 | 0.24 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 6 | 0.24 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 10 | 0.24 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 16 | 0.24 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 20 | 0.24 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 3 | 0.24 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 8 | 0.24 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 8 | 0.24 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 14 | 0.24 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 6 | 0.24 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 15 | 0.24 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 7 | 0.24 |
| (4,453) | 1:48:A:ILE:HG13 | 1:38:A:LEU:HA | 11 | 0.23 |
| (4,452) | 1:59:A:THR:HB | 1:59:A:THR:HG22 | 3 | 0.23 |
| (4,452) | 1:59:A:THR:HB | 1:59:A:THR:HG22 | 4 | 0.23 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 20 | 0.23 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 4 | 0.23 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 3 | 0.23 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 18 | 0.23 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 19 | 0.23 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 5 | 0.23 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 15 | 0.23 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 19 | 0.23 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 19 | 0.23 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 9 | 0.23 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 19 | 0.23 |
| (4,364) | 1:4:A:MET:HE3 | 1:58:A:GLU:HG3 | 10 | 0.23 |
| (4,300) | 1:97:A:LEU:HD23 | 1:156:A:PHE:HB3 | 14 | 0.23 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 8 | 0.23 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 13 | 0.23 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 15 | 0.23 |
| (4,254) | 1:41:A:MET:HE2 | 1:14:A:VAL:H | 20 | 0.23 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 16 | 0.23 |
| (4,208) | 1:14:A:VAL:HG22 | 1:11:A:LEU:HA | 14 | 0.23 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD13 | 6 | 0.23 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 8 | 0.23 |
| (4,9) | 1:22:A:ILE:HD13 | 1:10:A:PHE:HD1 | 20 | 0.23 |
| (4,6) | 1:10:A:PHE:HD1 | 1:21:A:LEU:HD22 | 12 | 0.23 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 6 | 0.23 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 4 | 0.23 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 16 | 0.23 |
| (2,3841) | 1:76:A:ALA:HB1 | 1:76:A:ALA:H | 1 | 0.23 |
| (2,3841) | 1:76:A:ALA:HB1 | 1:76:A:ALA:H | 2 | 0.23 |
| (2,3841) | 1:76:A:ALA:HB1 | 1:76:A:ALA:H | 17 | 0.23 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 11 | 0.23 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 7 | 0.23 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 13 | 0.23 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 16 | 0.23 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 15 | 0.23 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 16 | 0.23 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 3 | 0.23 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 20 | 0.23 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 4 | 0.23 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 6 | 0.23 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 4 | 0.23 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 1 | 0.23 |
| (2,3800) | 1:56:A:ILE:HD11 | 1:56:A:ILE:HG12 | 1 | 0.23 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 4 | 0.23 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 5 | 0.23 |
| (2,3789) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HB3 | 18 | 0.23 |
| (2,3781) | 1:142:A:VAL:HG13 | 1:142:A:VAL:HB | 12 | 0.23 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 1 | 0.23 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 2 | 0.23 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB3 | 7 | 0.23 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 9 | 0.23 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 11 | 0.23 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 13 | 0.23 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 14 | 0.23 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 19 | 0.23 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 20 | 0.23 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 5 | 0.23 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 7 | 0.23 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 9 | 0.23 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 20 | 0.23 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 5 | 0.23 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 7 | 0.23 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 6 | 0.23 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 11 | 0.23 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 4 | 0.23 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 19 | 0.23 |
| (2,3575) | 1:50:A:MET:HE1 | 1:50:A:MET:HG3 | 19 | 0.23 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 13 | 0.23 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 3 | 0.23 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 11 | 0.23 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 10 | 0.23 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 4 | 0.23 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 18 | 0.23 |
| (2,3495) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 10 | 0.23 |
| (2,3495) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 11 | 0.23 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 16 | 0.23 |
| (2,3495) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 17 | 0.23 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 18 | 0.23 |
| (2,3490) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HA | 20 | 0.23 |
| (2,3484) | 1:124:A:LEU:HD12 | 1:167:A:LEU:HA | 1 | 0.23 |
| (2,3484) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 18 | 0.23 |
| (2,3479) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 4 | 0.23 |
| (2,3479) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 9 | 0.23 |
| (2,3479) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 11 | 0.23 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 11 | 0.23 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 4 | 0.23 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 5 | 0.23 |
| (2,3372) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 10 | 0.23 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 16 | 0.23 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 8 | 0.23 |
| (2,3346) | 1:4:A:MET:HE1 | 1:55:A:HIS:HD2 | 5 | 0.23 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 20 | 0.23 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 5 | 0.23 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 10 | 0.23 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 13 | 0.23 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 19 | 0.23 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 10 | 0.23 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 15 | 0.23 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 20 | 0.23 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 17 | 0.23 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 8 | 0.23 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 11 | 0.23 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 17 | 0.23 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 2 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 9 | 0.23 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 11 | 0.23 |
| (2,2417) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 13 | 0.23 |
| (2,2376) | 1:95:A:ALA:HB1 | 1:149:A:LYS:H | 17 | 0.23 |
| (2,2348) | 1:156:A:PHE:H | 1:168:A:ILE:HD12 | 3 | 0.23 |
| (2,2308) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 8 | 0.23 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 7 | 0.23 |
| (2,2175) | 1:57:A:VAL:HG22 | 1:66:A:ALA:H | 4 | 0.23 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 16 | 0.23 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 5 | 0.23 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 18 | 0.23 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 8 | 0.23 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 6 | 0.23 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 19 | 0.23 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 3 | 0.23 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 17 | 0.23 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 9 | 0.23 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 14 | 0.23 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 16 | 0.23 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 20 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 2 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 3 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 4 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 9 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 10 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 13 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 15 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 16 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 17 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 18 | 0.23 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 19 | 0.23 |
| (2,1874) | 1:168:A:ILE:HD12 | 1:171:A:VAL:HG11 | 12 | 0.23 |
| (2,1874) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 15 | 0.23 |
| (2,1865) | 1:109:A:ILE:HD13 | 1:144:A:LEU:HD12 | 8 | 0.23 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 3 | 0.23 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 19 | 0.23 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 8 | 0.23 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 18 | 0.23 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 4 | 0.23 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 6 | 0.23 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 11 | 0.23 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 15 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1848) | 1:146:A:VAL:HG12 | 1:168:A:ILE:HD13 | 15 | 0.23 |
| (2,1844) | 1:110:A:LEU:HD23 | 1:110:A:LEU:HB3 | 1 | 0.23 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 18 | 0.23 |
| (2,1839) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HG12 | 2 | 0.23 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 8 | 0.23 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 14 | 0.23 |
| (2,1804) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HB | 10 | 0.23 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 19 | 0.23 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 20 | 0.23 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 10 | 0.23 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 3 | 0.23 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 10 | 0.23 |
| (2,1754) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 6 | 0.23 |
| (2,1754) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 9 | 0.23 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 5 | 0.23 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 12 | 0.23 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 2 | 0.23 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 3 | 0.23 |
| (2,1709) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HA | 5 | 0.23 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 9 | 0.23 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 10 | 0.23 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 11 | 0.23 |
| (2,1709) | 1:86:A:LEU:HD22 | 1:86:A:LEU:HA | 17 | 0.23 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 14 | 0.23 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 20 | 0.23 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 1 | 0.23 |
| (2,1576) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 17 | 0.23 |
| (2,1563) | 1:48:A:ILE:HG23 | 1:53:A:LEU:HB2 | 1 | 0.23 |
| (2,1536) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB3 | 20 | 0.23 |
| (2,1524) | 1:82:A:VAL:HG13 | 1:82:A:VAL:HA | 7 | 0.23 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 9 | 0.23 |
| (2,1524) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 10 | 0.23 |
| (2,1524) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 11 | 0.23 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 16 | 0.23 |
| (2,1494) | 1:168:A:ILE:HD12 | 1:156:A:PHE:HB2 | 17 | 0.23 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 10 | 0.23 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 13 | 0.23 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 14 | 0.23 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 17 | 0.23 |
| (2,1410) | 1:95:A:ALA:HB3 | 1:96:A:VAL:H | 7 | 0.23 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 10 | 0.23 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 18 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 20 | 0.23 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 11 | 0.23 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 13 | 0.23 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 19 | 0.23 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 2 | 0.23 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 5 | 0.23 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 10 | 0.23 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 14 | 0.23 |
| (2,1309) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HB3 | 20 | 0.23 |
| (2,1301) | 1:34:A:VAL:HG12 | 1:38:A:LEU:H | 16 | 0.23 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 6 | 0.23 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 7 | 0.23 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 20 | 0.23 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 9 | 0.23 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 14 | 0.23 |
| (2,1222) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 18 | 0.23 |
| (2,1218) | 1:177:A:LYS:HG2 | 1:177:A:LYS:HA | 2 | 0.23 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 9 | 0.23 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 11 | 0.23 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 14 | 0.23 |
| (2,1172) | 1:144:A:LEU:HD11 | 1:106:A:PHE:HE1 | 12 | 0.23 |
| (2,1131) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 18 | 0.23 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 1 | 0.23 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 3 | 0.23 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 11 | 0.23 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 12 | 0.23 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 14 | 0.23 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 8 | 0.23 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 11 | 0.23 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 13 | 0.23 |
| (2,977) | 1:87:A:GLY:H | 1:88:A:TYR:H | 6 | 0.23 |
| (2,943) | 1:159:A:TYR:H | 1:88:A:TYR:HD1 | 18 | 0.23 |
| (2,935) | 1:114:A:ILE:H | 1:171:A:VAL:H | 20 | 0.23 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 11 | 0.23 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 2 | 0.23 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD13 | 2 | 0.23 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD11 | 14 | 0.23 |
| (2,726) | 1:20:A:ALA:HB2 | 1:23:A:GLY:H | 1 | 0.23 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 17 | 0.23 |
| (2,653) | 1:29:A:ASN:H | 1:29:A:ASN:HB3 | 1 | 0.23 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 5 | 0.23 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 13 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,588) | 1:17:A:HIS:H | 1:16:A:ARG:HB2 | 19 | 0.23 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 1 | 0.23 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 4 | 0.23 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 11 | 0.23 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 15 | 0.23 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 18 | 0.23 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 20 | 0.23 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 2 | 0.23 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 5 | 0.23 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 10 | 0.23 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 18 | 0.23 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 2 | 0.23 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 5 | 0.23 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 11 | 0.23 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 13 | 0.23 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 15 | 0.23 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 18 | 0.23 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 11 | 0.23 |
| (2,375) | 1:156:A:PHE:H | 1:156:A:PHE:HD1 | 9 | 0.23 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 8 | 0.23 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 5 | 0.23 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 14 | 0.23 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 8 | 0.23 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 16 | 0.23 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 20 | 0.23 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 4 | 0.23 |
| (2,164) | 1:86:A:LEU:H | 1:86:A:LEU:HB3 | 20 | 0.23 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 11 | 0.23 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 11 | 0.23 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 9 | 0.23 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 2 | 0.23 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 16 | 0.23 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 16 | 0.23 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 2 | 0.23 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 5 | 0.23 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 10 | 0.23 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 3 | 0.23 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 7 | 0.23 |
| (1,118) | 1:168:A:ILE:N | 1:122:A:VAL:O | 1 | 0.23 |
| (1,118) | 1:168:A:ILE:N | 1:122:A:VAL:O | 15 | 0.23 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 4 | 0.23 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 12 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 4 | 0.23 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 14 | 0.23 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 13 | 0.23 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 19 | 0.23 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 14 | 0.23 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 19 | 0.23 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 12 | 0.23 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 20 | 0.23 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 1 | 0.23 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 10 | 0.23 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 13 | 0.23 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 14 | 0.23 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 15 | 0.23 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 8 | 0.23 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 10 | 0.23 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 11 | 0.23 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 14 | 0.23 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 19 | 0.23 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 4 | 0.23 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 17 | 0.23 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 6 | 0.23 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 7 | 0.23 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 12 | 0.23 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 20 | 0.23 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 16 | 0.23 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 1 | 0.23 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 9 | 0.23 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 1 | 0.23 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 2 | 0.23 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 3 | 0.23 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 3 | 0.23 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 5 | 0.23 |
| (4,453) | 1:48:A:ILE:HG13 | 1:38:A:LEU:HA | 16 | 0.22 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 8 | 0.22 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 18 | 0.22 |
| (4,451) | 1:168:A:ILE:HD13 | 1:168:A:ILE:HG12 | 14 | 0.22 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 10 | 0.22 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 2 | 0.22 |
| (4,410) | 1:50:A:MET:HE3 | 1:54:A:LYS:HD3 | 2 | 0.22 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 1 | 0.22 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 2 | 0.22 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 18 | 0.22 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 7 | 0.22 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 13 | 0.22 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 20 | 0.22 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 1 | 0.22 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 3 | 0.22 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 8 | 0.22 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 11 | 0.22 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 14 | 0.22 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 15 | 0.22 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 17 | 0.22 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 8 | 0.22 |
| (4,208) | 1:14:A:VAL:HG22 | 1:11:A:LEU:HA | 10 | 0.22 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 11 | 0.22 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 9 | 0.22 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 18 | 0.22 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 3 | 0.22 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 9 | 0.22 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 14 | 0.22 |
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 19 | 0.22 |
| (2,3836) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 11 | 0.22 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 19 | 0.22 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 9 | 0.22 |
| (2,3824) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 16 | 0.22 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 3 | 0.22 |
| (2,3819) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 2 | 0.22 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 14 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 1 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 8 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 9 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 10 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 12 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG22 | 13 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG23 | 1:14:A:VAL:HG21 | 16 | 0.22 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 17 | 0.22 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 2 | 0.22 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 5 | 0.22 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG22 | 13 | 0.22 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 16 | 0.22 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 19 | 0.22 |
| (2,3813) | 1:56:A:ILE:HD11 | 1:11:A:LEU:HD11 | 8 | 0.22 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 10 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 16 | 0.22 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 10 | 0.22 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 12 | 0.22 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 15 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 2 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 3 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD12 | 1:56:A:ILE:HG12 | 4 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD12 | 1:56:A:ILE:HG12 | 5 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 10 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 14 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 15 | 0.22 |
| (2,3800) | 1:56:A:ILE:HD13 | 1:56:A:ILE:HG12 | 18 | 0.22 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 9 | 0.22 |
| (2,3795) | 1:14:A:VAL:HG23 | 1:21:A:LEU:HG | 11 | 0.22 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 9 | 0.22 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 16 | 0.22 |
| (2,3765) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 18 | 0.22 |
| (2,3760) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 5 | 0.22 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 7 | 0.22 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 16 | 0.22 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 13 | 0.22 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 16 | 0.22 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 19 | 0.22 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 12 | 0.22 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 17 | 0.22 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 10 | 0.22 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 16 | 0.22 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 2 | 0.22 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 8 | 0.22 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 9 | 0.22 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 17 | 0.22 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 15 | 0.22 |
| (2,3570) | 1:4:A:MET:HE3 | 1:52:A:GLU:HA | 15 | 0.22 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE1 | 7 | 0.22 |
| (2,3558) | 1:152:A:ALA:HB2 | 1:149:A:LYS:HA | 14 | 0.22 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 11 | 0.22 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 20 | 0.22 |
| (2,3531) | 1:151:A:MET:HE1 | 1:175:A:PHE:HB3 | 11 | 0.22 |
| (2,3527) | 1:84:A:VAL:HG21 | 1:85:A:ASP:HB2 | 8 | 0.22 |
| (2,3509) | 1:13:A:LEU:HD21 | 1:17:A:HIS:HB2 | 10 | 0.22 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 3 | 0.22 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 4 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 6 | 0.22 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 12 | 0.22 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 6 | 0.22 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 10 | 0.22 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 11 | 0.22 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 13 | 0.22 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 15 | 0.22 |
| (2,3495) | 1:82:A:VAL:HG13 | 1:82:A:VAL:HA | 7 | 0.22 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 9 | 0.22 |
| (2,3495) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 15 | 0.22 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 5 | 0.22 |
| (2,3467) | 1:11:A:LEU:HD12 | 1:38:A:LEU:HA | 14 | 0.22 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 15 | 0.22 |
| (2,3452) | 1:168:A:ILE:HD13 | 1:156:A:PHE:HZ | 11 | 0.22 |
| (2,3439) | 1:110:A:LEU:HD12 | 1:110:A:LEU:H | 19 | 0.22 |
| (2,3434) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HE1 | 1 | 0.22 |
| (2,3434) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HE1 | 11 | 0.22 |
| (2,3391) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 3 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 1 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 4 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 6 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 7 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 11 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 14 | 0.22 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 20 | 0.22 |
| (2,3345) | 1:41:A:MET:HE1 | 1:10:A:PHE:HE1 | 1 | 0.22 |
| (2,3345) | 1:41:A:MET:HE2 | 1:10:A:PHE:HE1 | 20 | 0.22 |
| (2,3265) | 1:84:A:VAL:HG11 | 1:84:A:VAL:H | 5 | 0.22 |
| (2,3265) | 1:84:A:VAL:HG12 | 1:84:A:VAL:H | 19 | 0.22 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB3 | 20 | 0.22 |
| (2,3182) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 14 | 0.22 |
| (2,3182) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 19 | 0.22 |
| (2,3167) | 1:176:A:ILE:HD12 | 1:114:A:ILE:HD13 | 6 | 0.22 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 16 | 0.22 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 8 | 0.22 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 14 | 0.22 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 18 | 0.22 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 10 | 0.22 |
| (2,2918) | 1:76:A:ALA:HB3 | 1:78:A:GLN:HE22 | 15 | 0.22 |
| (2,2657) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 9 | 0.22 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 8 | 0.22 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 5 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 7 | 0.22 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 16 | 0.22 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 12 | 0.22 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 3 | 0.22 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 5 | 0.22 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 8 | 0.22 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 14 | 0.22 |
| (2,2210) | 1:48:A:ILE:HD13 | 1:53:A:LEU:H | 4 | 0.22 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 6 | 0.22 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 9 | 0.22 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 6 | 0.22 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD11 | 4 | 0.22 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 14 | 0.22 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 3 | 0.22 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 4 | 0.22 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 5 | 0.22 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 6 | 0.22 |
| (2,2041) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 9 | 0.22 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 1 | 0.22 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 8 | 0.22 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 14 | 0.22 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 16 | 0.22 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 1 | 0.22 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 6 | 0.22 |
| (2,1898) | 1:24:A:LEU:HA | 1:24:A:LEU:HB3 | 20 | 0.22 |
| (2,1880) | 1:76:A:ALA:HB3 | 1:16:A:ARG:HA | 15 | 0.22 |
| (2,1869) | 1:97:A:LEU:HD23 | 1:96:A:VAL:HB | 5 | 0.22 |
| (2,1861) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 16 | 0.22 |
| (2,1857) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 17 | 0.22 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 2 | 0.22 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 14 | 0.22 |
| (2,1854) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 18 | 0.22 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 4 | 0.22 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 6 | 0.22 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 13 | 0.22 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 17 | 0.22 |
| (2,1800) | 1:53:A:LEU:HD13 | 1:37:A:LEU:HG | 10 | 0.22 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 12 | 0.22 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 14 | 0.22 |
| (2,1800) | 1:53:A:LEU:HD13 | 1:37:A:LEU:HG | 18 | 0.22 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 19 | 0.22 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 7 | 0.22 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 3 | 0.22 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 12 | 0.22 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 14 | 0.22 |
| (2,1599) | 1:4:A:MET:HE2 | 1:52:A:GLU:HA | 18 | 0.22 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 2 | 0.22 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 10 | 0.22 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 15 | 0.22 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 17 | 0.22 |
| (2,1549) | 1:37:A:LEU:HD12 | 1:41:A:MET:HG2 | 7 | 0.22 |
| (2,1524) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 15 | 0.22 |
| (2,1509) | 1:151:A:MET:HE3 | 1:171:A:VAL:HA | 14 | 0.22 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 5 | 0.22 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 12 | 0.22 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 11 | 0.22 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 13 | 0.22 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 15 | 0.22 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 12 | 0.22 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 16 | 0.22 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 13 | 0.22 |
| (2,1294) | 1:57:A:VAL:HG11 | 1:58:A:GLU:H | 18 | 0.22 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 1 | 0.22 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 14 | 0.22 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 1 | 0.22 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 3 | 0.22 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD13 | 15 | 0.22 |
| (2,1218) | 1:177:A:LYS:HG2 | 1:177:A:LYS:HA | 11 | 0.22 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 2 | 0.22 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 3 | 0.22 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 6 | 0.22 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 7 | 0.22 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 8 | 0.22 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 17 | 0.22 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 19 | 0.22 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 20 | 0.22 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 2 | 0.22 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 4 | 0.22 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 5 | 0.22 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 8 | 0.22 |
| (2,1172) | 1:144:A:LEU:HD11 | 1:106:A:PHE:HE1 | 9 | 0.22 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 4 | 0.22 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 16 | 0.22 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 20 | 0.22 |
| (2,1155) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 12 | 0.22 |
| (2,1131) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 19 | 0.22 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 6 | 0.22 |
| (2,1067) | 1:56:A:ILE:H | 1:55:A:HIS:H | 20 | 0.22 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 7 | 0.22 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 17 | 0.22 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 1 | 0.22 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD11 | 11 | 0.22 |
| (2,780) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 3 | 0.22 |
| (2,692) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 14 | 0.22 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 9 | 0.22 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 13 | 0.22 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 16 | 0.22 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 1 | 0.22 |
| (2,594) | 1:43:A:ALA:HB3 | 1:44:A:LYS:H | 15 | 0.22 |
| (2,550) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 10 | 0.22 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 6 | 0.22 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 8 | 0.22 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 3 | 0.22 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 5 | 0.22 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 8 | 0.22 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 16 | 0.22 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 3 | 0.22 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 11 | 0.22 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 12 | 0.22 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 6 | 0.22 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 1 | 0.22 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 9 | 0.22 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 10 | 0.22 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 12 | 0.22 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 14 | 0.22 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 19 | 0.22 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 6 | 0.22 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 2 | 0.22 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 11 | 0.22 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 6 | 0.22 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 11 | 0.22 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 2 | 0.22 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 3 | 0.22 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 5 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 9 | 0.22 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 17 | 0.22 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 2 | 0.22 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 19 | 0.22 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 15 | 0.22 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 7 | 0.22 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 2 | 0.22 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 4 | 0.22 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 6 | 0.22 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 10 | 0.22 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 19 | 0.22 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 10 | 0.22 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 16 | 0.22 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 9 | 0.22 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 7 | 0.22 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 3 | 0.22 |
| (1,112) | 1:159:A:TYR:N | 1:167:A:LEU:O | 10 | 0.22 |
| (1,112) | 1:159:A:TYR:N | 1:167:A:LEU:O | 11 | 0.22 |
| (1,112) | 1:159:A:TYR:N | 1:167:A:LEU:O | 15 | 0.22 |
| (1,112) | 1:159:A:TYR:N | 1:167:A:LEU:O | 19 | 0.22 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 1 | 0.22 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 5 | 0.22 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 7 | 0.22 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 15 | 0.22 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 17 | 0.22 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 18 | 0.22 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 2 | 0.22 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 14 | 0.22 |
| (1,92) | 1:133:A:LYS:N | 1:129:A:THR:O | 14 | 0.22 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 16 | 0.22 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 2 | 0.22 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 3 | 0.22 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 9 | 0.22 |
| (1,77) | 1:112:A:ASP:H | 1:108:A:LEU:O | 5 | 0.22 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 12 | 0.22 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 17 | 0.22 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 18 | 0.22 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 13 | 0.22 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 18 | 0.22 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 7 | 0.22 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 11 | 0.22 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 20 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 2 | 0.22 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 5 | 0.22 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 9 | 0.22 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 5 | 0.22 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 17 | 0.22 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 5 | 0.22 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 8 | 0.22 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 2 | 0.22 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 8 | 0.22 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 18 | 0.22 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 9 | 0.22 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 11 | 0.22 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 15 | 0.22 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 19 | 0.22 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 2 | 0.22 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 7 | 0.22 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 11 | 0.22 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 13 | 0.22 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 15 | 0.22 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 17 | 0.22 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 19 | 0.22 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 20 | 0.22 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 10 | 0.22 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 12 | 0.22 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 13 | 0.22 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 14 | 0.22 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 19 | 0.22 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 9 | 0.22 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 13 | 0.22 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 17 | 0.22 |
| (1,4) | 1:8:A:SER:N | 1:4:A:MET:O | 15 | 0.22 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 7 | 0.21 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 10 | 0.21 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 16 | 0.21 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 19 | 0.21 |
| (4,446) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 1 | 0.21 |
| (4,445) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 2 | 0.21 |
| (4,443) | 1:48:A:ILE:HD12 | 1:38:A:LEU:HB2 | 5 | 0.21 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 1 | 0.21 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 13 | 0.21 |
| (4,411) | 1:84:A:VAL:HB | 1:86:A:LEU:HB3 | 17 | 0.21 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 6 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 9 | 0.21 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 11 | 0.21 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 16 | 0.21 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 17 | 0.21 |
| (4,395) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 8 | 0.21 |
| (4,395) | 1:56:A:ILE:HG22 | 1:56:A:ILE:HA | 9 | 0.21 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 4 | 0.21 |
| (4,379) | 1:50:A:MET:HA | 1:39:A:ALA:HB3 | 8 | 0.21 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 8 | 0.21 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 11 | 0.21 |
| (4,307) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 19 | 0.21 |
| (4,307) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 20 | 0.21 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 14 | 0.21 |
| (4,259) | 1:117:A:MET:HE3 | 2:201:A:NAD:H2A | 8 | 0.21 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 2 | 0.21 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 4 | 0.21 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 5 | 0.21 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 6 | 0.21 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 9 | 0.21 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 10 | 0.21 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 20 | 0.21 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 19 | 0.21 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 7 | 0.21 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 7 | 0.21 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 20 | 0.21 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD23 | 2 | 0.21 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 10 | 0.21 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 6 | 0.21 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 10 | 0.21 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 17 | 0.21 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 20 | 0.21 |
| (2,3841) | 1:76:A:ALA:HB1 | 1:76:A:ALA:H | 14 | 0.21 |
| (2,3841) | 1:76:A:ALA:HB1 | 1:76:A:ALA:H | 16 | 0.21 |
| (2,3829) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 5 | 0.21 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 2 | 0.21 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 15 | 0.21 |
| (2,3823) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB | 2 | 0.21 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 3 | 0.21 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 4 | 0.21 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 6 | 0.21 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 7 | 0.21 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 11 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG21 | 19 | 0.21 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 18 | 0.21 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 18 | 0.21 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 2 | 0.21 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 6 | 0.21 |
| (2,3805) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HB | 18 | 0.21 |
| (2,3800) | 1:56:A:ILE:HD11 | 1:56:A:ILE:HG12 | 8 | 0.21 |
| (2,3800) | 1:56:A:ILE:HD12 | 1:56:A:ILE:HG12 | 11 | 0.21 |
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 14 | 0.21 |
| (2,3795) | 1:14:A:VAL:HG21 | 1:21:A:LEU:HG | 12 | 0.21 |
| (2,3795) | 1:14:A:VAL:HG22 | 1:21:A:LEU:HG | 13 | 0.21 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 10 | 0.21 |
| (2,3786) | 1:38:A:LEU:HG | 1:38:A:LEU:HD12 | 16 | 0.21 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 20 | 0.21 |
| (2,3770) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 1 | 0.21 |
| (2,3763) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD12 | 2 | 0.21 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 8 | 0.21 |
| (2,3763) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD12 | 10 | 0.21 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 6 | 0.21 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG21 | 14 | 0.21 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 1 | 0.21 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 4 | 0.21 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 15 | 0.21 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 17 | 0.21 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 12 | 0.21 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 20 | 0.21 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 1 | 0.21 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 10 | 0.21 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 13 | 0.21 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 18 | 0.21 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 5 | 0.21 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 6 | 0.21 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 10 | 0.21 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 12 | 0.21 |
| (2,3653) | 1:14:A:VAL:HG23 | 1:19:A:PRO:HA | 20 | 0.21 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 4 | 0.21 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 19 | 0.21 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 4 | 0.21 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 7 | 0.21 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 13 | 0.21 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 11 | 0.21 |
| (2,3524) | 1:13:A:LEU:HD13 | 1:18:A:ASN:HB2 | 14 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 9 | 0.21 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 11 | 0.21 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 13 | 0.21 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 17 | 0.21 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 8 | 0.21 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 9 | 0.21 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 14 | 0.21 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 19 | 0.21 |
| (2,3495) | 1:82:A:VAL:HG12 | 1:82:A:VAL:HA | 5 | 0.21 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 6 | 0.21 |
| (2,3430) | 1:128:A:ILE:HD12 | 1:127:A:ASP:H | 13 | 0.21 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 7 | 0.21 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 19 | 0.21 |
| (2,3387) | 1:21:A:LEU:HD22 | 1:10:A:PHE:HE1 | 8 | 0.21 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 2 | 0.21 |
| (2,3372) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 3 | 0.21 |
| (2,3372) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 12 | 0.21 |
| (2,3372) | 1:20:A:ALA:HB3 | 1:20:A:ALA:H | 13 | 0.21 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 17 | 0.21 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 18 | 0.21 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 19 | 0.21 |
| (2,3345) | 1:41:A:MET:HE1 | 1:10:A:PHE:HE1 | 3 | 0.21 |
| (2,3288) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 12 | 0.21 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 4 | 0.21 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 12 | 0.21 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 2 | 0.21 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 12 | 0.21 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 13 | 0.21 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 1 | 0.21 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 4 | 0.21 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 7 | 0.21 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 12 | 0.21 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 15 | 0.21 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 18 | 0.21 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 20 | 0.21 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 6 | 0.21 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 13 | 0.21 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 19 | 0.21 |
| (2,2994) | 1:84:A:VAL:H | 1:83:A:GLU:H | 9 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 1 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD22 | 6 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 7 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 13 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 15 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 18 | 0.21 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 19 | 0.21 |
| (2,2680) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 6 | 0.21 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 11 | 0.21 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 12 | 0.21 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 15 | 0.21 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 20 | 0.21 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 4 | 0.21 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 9 | 0.21 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 13 | 0.21 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 17 | 0.21 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG11 | 1 | 0.21 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 17 | 0.21 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 7 | 0.21 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 9 | 0.21 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 19 | 0.21 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 18 | 0.21 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 4 | 0.21 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 15 | 0.21 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD11 | 19 | 0.21 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 15 | 0.21 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 17 | 0.21 |
| (2,1967) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 17 | 0.21 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 9 | 0.21 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 12 | 0.21 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 20 | 0.21 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 12 | 0.21 |
| (2,1884) | 1:41:A:MET:HE2 | 1:46:A:HIS:HA | 12 | 0.21 |
| (2,1871) | 1:97:A:LEU:HD21 | 1:151:A:MET:HG3 | 4 | 0.21 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 17 | 0.21 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 2 | 0.21 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 9 | 0.21 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 12 | 0.21 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 18 | 0.21 |
| (2,1857) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 12 | 0.21 |
| (2,1844) | 1:110:A:LEU:HD22 | 1:110:A:LEU:HB3 | 7 | 0.21 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 3 | 0.21 |
| (2,1804) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HB | 5 | 0.21 |
| (2,1804) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HB | 16 | 0.21 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 2 | 0.21 |
| (2,1800) | 1:53:A:LEU:HD13 | 1:37:A:LEU:HG | 6 | 0.21 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 4 | 0.21 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 11 | 0.21 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 1 | 0.21 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 13 | 0.21 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 12 | 0.21 |
| (2,1599) | 1:4:A:MET:HE3 | 1:52:A:GLU:HA | 1 | 0.21 |
| (2,1594) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE1 | 18 | 0.21 |
| (2,1524) | 1:82:A:VAL:HG12 | 1:82:A:VAL:HA | 5 | 0.21 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 6 | 0.21 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 19 | 0.21 |
| (2,1514) | 1:124:A:LEU:HD12 | 1:167:A:LEU:HA | 1 | 0.21 |
| (2,1514) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 18 | 0.21 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 2 | 0.21 |
| (2,1474) | 1:110:A:LEU:HD21 | 1:110:A:LEU:H | 17 | 0.21 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 4 | 0.21 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 6 | 0.21 |
| (2,1420) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HE1 | 19 | 0.21 |
| (2,1417) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HZ | 5 | 0.21 |
| (2,1412) | 1:66:A:ALA:HB2 | 1:31:A:TRP:HZ3 | 15 | 0.21 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 11 | 0.21 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 3 | 0.21 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 6 | 0.21 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 19 | 0.21 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 9 | 0.21 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 6 | 0.21 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 20 | 0.21 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 17 | 0.21 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 1 | 0.21 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 5 | 0.21 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 10 | 0.21 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 13 | 0.21 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 15 | 0.21 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 16 | 0.21 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 18 | 0.21 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 3 | 0.21 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 9 | 0.21 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 5 | 0.21 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 9 | 0.21 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 11 | 0.21 |
| (2,1131) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 16 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 8 | 0.21 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 17 | 0.21 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 2 | 0.21 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 2 | 0.21 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 8 | 0.21 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 11 | 0.21 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 13 | 0.21 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 15 | 0.21 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 17 | 0.21 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD11 | 4 | 0.21 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD11 | 10 | 0.21 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD11 | 16 | 0.21 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 5 | 0.21 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 2 | 0.21 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 1 | 0.21 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 16 | 0.21 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 4 | 0.21 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 5 | 0.21 |
| (2,594) | 1:43:A:ALA:HB1 | 1:44:A:LYS:H | 12 | 0.21 |
| (2,550) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 4 | 0.21 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 9 | 0.21 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 12 | 0.21 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 2 | 0.21 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 13 | 0.21 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 14 | 0.21 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 1 | 0.21 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 20 | 0.21 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 3 | 0.21 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 8 | 0.21 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 16 | 0.21 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 20 | 0.21 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 13 | 0.21 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 18 | 0.21 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 8 | 0.21 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 14 | 0.21 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 1 | 0.21 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 6 | 0.21 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 1 | 0.21 |
| (2,342) | 1:41:A:MET:H | 1:41:A:MET:HG2 | 5 | 0.21 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 17 | 0.21 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 4 | 0.21 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 7 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 9 | 0.21 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 18 | 0.21 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 19 | 0.21 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 9 | 0.21 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 10 | 0.21 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 12 | 0.21 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 13 | 0.21 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 20 | 0.21 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 7 | 0.21 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 3 | 0.21 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 10 | 0.21 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 17 | 0.21 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 4 | 0.21 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 10 | 0.21 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 20 | 0.21 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 1 | 0.21 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 5 | 0.21 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 17 | 0.21 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 20 | 0.21 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 3 | 0.21 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 10 | 0.21 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 9 | 0.21 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 11 | 0.21 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 17 | 0.21 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 6 | 0.21 |
| (1,118) | 1:168:A:ILE:N | 1:122:A:VAL:O | 19 | 0.21 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 5 | 0.21 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 19 | 0.21 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 13 | 0.21 |
| (1,114) | 1:166:A:TRP:N | 1:124:A:LEU:O | 14 | 0.21 |
| (1,112) | 1:159:A:TYR:N | 1:167:A:LEU:O | 9 | 0.21 |
| (1,112) | 1:159:A:TYR:N | 1:167:A:LEU:O | 18 | 0.21 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 16 | 0.21 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 9 | 0.21 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 4 | 0.21 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 12 | 0.21 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 16 | 0.21 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 20 | 0.21 |
| (1,92) | 1:133:A:LYS:N | 1:129:A:THR:O | 2 | 0.21 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 10 | 0.21 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 12 | 0.21 |
| (1,88) | 1:131:A:ALA:N | 1:127:A:ASP:O | 15 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 7 | 0.21 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 8 | 0.21 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 11 | 0.21 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 14 | 0.21 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 17 | 0.21 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 18 | 0.21 |
| (1,77) | 1:112:A:ASP:H | 1:108:A:LEU:O | 20 | 0.21 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 5 | 0.21 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 9 | 0.21 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 13 | 0.21 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 1 | 0.21 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 4 | 0.21 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 14 | 0.21 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 6 | 0.21 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 5 | 0.21 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 16 | 0.21 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 17 | 0.21 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 3 | 0.21 |
| (1,51) | 1:60:A:ASN:H | 1:56:A:ILE:O | 17 | 0.21 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 13 | 0.21 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 14 | 0.21 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 20 | 0.21 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 10 | 0.21 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 13 | 0.21 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 15 | 0.21 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 2 | 0.21 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 7 | 0.21 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 12 | 0.21 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 17 | 0.21 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 17 | 0.21 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 8 | 0.21 |
| (1,16) | 1:14:A:VAL:N | 1:10:A:PHE:O | 1 | 0.21 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 2 | 0.21 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 7 | 0.21 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 15 | 0.21 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 17 | 0.21 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 4 | 0.21 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 10 | 0.21 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 16 | 0.21 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 20 | 0.21 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 16 | 0.21 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 18 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 11 | 0.2 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 6 | 0.2 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 10 | 0.2 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 2 | 0.2 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 3 | 0.2 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 4 | 0.2 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 7 | 0.2 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 10 | 0.2 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 12 | 0.2 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 14 | 0.2 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 20 | 0.2 |
| (4,392) | 1:8:A:SER:HB2 | 1:7:A:VAL:HB | 16 | 0.2 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 3 | 0.2 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 16 | 0.2 |
| (4,328) | 1:171:A:VAL:HG12 | 1:113:A:GLY:HA2 | 5 | 0.2 |
| (4,325) | 1:7:A:VAL:HG13 | 1:10:A:PHE:HB3 | 1 | 0.2 |
| (4,325) | 1:7:A:VAL:HG11 | 1:10:A:PHE:HB3 | 3 | 0.2 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 17 | 0.2 |
| (4,283) | 1:142:A:VAL:HG13 | 1:103:A:GLU:H | 9 | 0.2 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 17 | 0.2 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 7 | 0.2 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 13 | 0.2 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 19 | 0.2 |
| (4,213) | 1:143:A:VAL:HB | 1:144:A:LEU:HA | 18 | 0.2 |
| (4,208) | 1:14:A:VAL:HG22 | 1:11:A:LEU:HA | 7 | 0.2 |
| (4,208) | 1:14:A:VAL:HG22 | 1:11:A:LEU:HA | 9 | 0.2 |
| (4,208) | 1:14:A:VAL:HG22 | 1:11:A:LEU:HA | 15 | 0.2 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 16 | 0.2 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 19 | 0.2 |
| (4,198) | 1:176:A:ILE:HD13 | 1:106:A:PHE:HE1 | 2 | 0.2 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 9 | 0.2 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 12 | 0.2 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 2 | 0.2 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 20 | 0.2 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 5 | 0.2 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 11 | 0.2 |
| (2,3940) | 1:134:A:VAL:HG11 | 2:201:A:NAD:H2N | 7 | 0.2 |
| (2,3940) | 1:134:A:VAL:HG11 | 2:201:A:NAD:H2N | 15 | 0.2 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 2 | 0.2 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 5 | 0.2 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 13 | 0.2 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 19 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 4 | 0.2 |
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 6 | 0.2 |
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 8 | 0.2 |
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 12 | 0.2 |
| (2,3836) | 1:168:A:ILE:HD11 | 1:171:A:VAL:HG11 | 7 | 0.2 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 2 | 0.2 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 8 | 0.2 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 17 | 0.2 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 2 | 0.2 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 9 | 0.2 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 12 | 0.2 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 18 | 0.2 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG22 | 1 | 0.2 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 7 | 0.2 |
| (2,3819) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 4 | 0.2 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 2 | 0.2 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 15 | 0.2 |
| (2,3800) | 1:56:A:ILE:HD12 | 1:56:A:ILE:HG12 | 12 | 0.2 |
| (2,3793) | 1:53:A:LEU:HD22 | 1:56:A:ILE:HB | 6 | 0.2 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 14 | 0.2 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 17 | 0.2 |
| (2,3789) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HB3 | 19 | 0.2 |
| (2,3785) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 18 | 0.2 |
| (2,3763) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD12 | 18 | 0.2 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 1 | 0.2 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 2 | 0.2 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 3 | 0.2 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 5 | 0.2 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 11 | 0.2 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 15 | 0.2 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 3 | 0.2 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 8 | 0.2 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 14 | 0.2 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 5 | 0.2 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 4 | 0.2 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 15 | 0.2 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 19 | 0.2 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 7 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 2 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 3 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 7 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 11 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG23 | 1:19:A:PRO:HA | 13 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 16 | 0.2 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 18 | 0.2 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 14 | 0.2 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 5 | 0.2 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 6 | 0.2 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 8 | 0.2 |
| (2,3558) | 1:152:A:ALA:HB2 | 1:149:A:LYS:HA | 2 | 0.2 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 1 | 0.2 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 2 | 0.2 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 6 | 0.2 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 12 | 0.2 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 12 | 0.2 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 15 | 0.2 |
| (2,3531) | 1:151:A:MET:HE1 | 1:175:A:PHE:HB3 | 6 | 0.2 |
| (2,3527) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 10 | 0.2 |
| (2,3518) | 1:128:A:ILE:HD13 | 1:128:A:ILE:HA | 18 | 0.2 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 7 | 0.2 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 2 | 0.2 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 7 | 0.2 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 17 | 0.2 |
| (2,3498) | 1:38:A:LEU:HD23 | 1:47:A:GLY:HA2 | 12 | 0.2 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 19 | 0.2 |
| (2,3490) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HA | 4 | 0.2 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 9 | 0.2 |
| (2,3430) | 1:128:A:ILE:HD12 | 1:127:A:ASP:H | 7 | 0.2 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 1 | 0.2 |
| (2,3399) | 1:21:A:LEU:HD13 | 1:21:A:LEU:H | 1 | 0.2 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 8 | 0.2 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 14 | 0.2 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 8 | 0.2 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 15 | 0.2 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 11 | 0.2 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 14 | 0.2 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 18 | 0.2 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 18 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 1 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 3 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 4 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 5 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 6 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 10 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 14 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 15 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 19 | 0.2 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 20 | 0.2 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 16 | 0.2 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 1 | 0.2 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 4 | 0.2 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 5 | 0.2 |
| (2,3127) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD23 | 4 | 0.2 |
| (2,3127) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD23 | 19 | 0.2 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 4 | 0.2 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 9 | 0.2 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 12 | 0.2 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD22 | 16 | 0.2 |
| (2,2852) | 1:85:A:ASP:H | 1:86:A:LEU:H | 4 | 0.2 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 6 | 0.2 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 4 | 0.2 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 2 | 0.2 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 3 | 0.2 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 12 | 0.2 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 17 | 0.2 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 12 | 0.2 |
| (2,2521) | 1:105:A:ASN:H | 1:102:A:ALA:HB3 | 17 | 0.2 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 4 | 0.2 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 10 | 0.2 |
| (2,2308) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 11 | 0.2 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 6 | 0.2 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 10 | 0.2 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 18 | 0.2 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 12 | 0.2 |
| (2,2167) | 1:24:A:LEU:H | 1:14:A:VAL:HG11 | 11 | 0.2 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 9 | 0.2 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 18 | 0.2 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 19 | 0.2 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 20 | 0.2 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 15 | 0.2 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 8 | 0.2 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 1 | 0.2 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 7 | 0.2 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 19 | 0.2 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 4 | 0.2 |
| (2,1889) | 1:4:A:MET:HE1 | 1:4:A:MET:HA | 14 | 0.2 |
| (2,1871) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 18 | 0.2 |
| (2,1869) | 1:97:A:LEU:HD22 | 1:96:A:VAL:HB | 4 | 0.2 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 9 | 0.2 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 1 | 0.2 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 2 | 0.2 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 15 | 0.2 |
| (2,1861) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 20 | 0.2 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 3 | 0.2 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 4 | 0.2 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 17 | 0.2 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 19 | 0.2 |
| (2,1828) | 1:151:A:MET:HE1 | 1:151:A:MET:HG3 | 20 | 0.2 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 20 | 0.2 |
| (2,1807) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 1 | 0.2 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 3 | 0.2 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 5 | 0.2 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 9 | 0.2 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 15 | 0.2 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 19 | 0.2 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 20 | 0.2 |
| (2,1791) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 19 | 0.2 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 18 | 0.2 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 10 | 0.2 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 13 | 0.2 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 14 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 2 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 4 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 6 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 7 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 8 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 9 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 11 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 16 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 17 | 0.2 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 19 | 0.2 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 8 | 0.2 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 16 | 0.2 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 18 | 0.2 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 10 | 0.2 |
| (2,1563) | 1:48:A:ILE:HG23 | 1:53:A:LEU:HB2 | 17 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 12 | 0.2 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 3 | 0.2 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 11 | 0.2 |
| (2,1459) | 1:108:A:LEU:HD13 | 2:201:A:NAD:H2A | 6 | 0.2 |
| (2,1459) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 14 | 0.2 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 3 | 0.2 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 8 | 0.2 |
| (2,1420) | 1:22:A:ILE:HG21 | 1:10:A:PHE:HE1 | 20 | 0.2 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 6 | 0.2 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 20 | 0.2 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 3 | 0.2 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 4 | 0.2 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 7 | 0.2 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 15 | 0.2 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 3 | 0.2 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 13 | 0.2 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 19 | 0.2 |
| (2,1282) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 5 | 0.2 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 18 | 0.2 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 5 | 0.2 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 19 | 0.2 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 4 | 0.2 |
| (2,1199) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 12 | 0.2 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 10 | 0.2 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 12 | 0.2 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 15 | 0.2 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 17 | 0.2 |
| (2,1172) | 1:144:A:LEU:HD11 | 1:106:A:PHE:HE1 | 2 | 0.2 |
| (2,1172) | 1:144:A:LEU:HD11 | 1:106:A:PHE:HE1 | 4 | 0.2 |
| (2,1172) | 1:144:A:LEU:HD11 | 1:106:A:PHE:HE1 | 8 | 0.2 |
| (2,1172) | 1:144:A:LEU:HD11 | 1:106:A:PHE:HE1 | 18 | 0.2 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 6 | 0.2 |
| (2,1131) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 20 | 0.2 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 9 | 0.2 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 11 | 0.2 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 18 | 0.2 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 19 | 0.2 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 18 | 0.2 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 17 | 0.2 |
| (2,974) | 1:44:A:LYS:H | 1:45:A:GLY:H | 19 | 0.2 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 4 | 0.2 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 7 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 9 | 0.2 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 14 | 0.2 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 15 | 0.2 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 17 | 0.2 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 10 | 0.2 |
| (2,866) | 1:77:A:ASN:HD22 | 1:64:A:ARG:HA | 5 | 0.2 |
| (2,821) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 17 | 0.2 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 12 | 0.2 |
| (2,726) | 1:20:A:ALA:HB2 | 1:23:A:GLY:H | 13 | 0.2 |
| (2,718) | 1:91:A:GLN:HE21 | 1:89:A:GLU:HB2 | 13 | 0.2 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 7 | 0.2 |
| (2,684) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 2 | 0.2 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 2 | 0.2 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 4 | 0.2 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 7 | 0.2 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 17 | 0.2 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 18 | 0.2 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 5 | 0.2 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 11 | 0.2 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 18 | 0.2 |
| (2,594) | 1:43:A:ALA:HB3 | 1:44:A:LYS:H | 19 | 0.2 |
| (2,594) | 1:43:A:ALA:HB3 | 1:44:A:LYS:H | 20 | 0.2 |
| (2,549) | 1:8:A:SER:H | 1:6:A:LYS:HA | 12 | 0.2 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 6 | 0.2 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 13 | 0.2 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 19 | 0.2 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 4 | 0.2 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 7 | 0.2 |
| (2,472) | 1:110:A:LEU:H | 1:110:A:LEU:HA | 17 | 0.2 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 2 | 0.2 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 4 | 0.2 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 7 | 0.2 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 9 | 0.2 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 11 | 0.2 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 16 | 0.2 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 20 | 0.2 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 19 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 3 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 5 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 11 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 13 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 15 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 17 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 18 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 19 | 0.2 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 20 | 0.2 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 6 | 0.2 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 6 | 0.2 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 8 | 0.2 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 13 | 0.2 |
| (2,229) | 1:43:A:ALA:H | 1:42:A:LYS:HG3 | 14 | 0.2 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 15 | 0.2 |
| (2,224) | 1:81:A:SER:HA | 1:82:A:VAL:H | 15 | 0.2 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 15 | 0.2 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 18 | 0.2 |
| (2,190) | 1:13:A:LEU:H | 1:13:A:LEU:HB3 | 12 | 0.2 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 4 | 0.2 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 6 | 0.2 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 7 | 0.2 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 10 | 0.2 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 11 | 0.2 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 18 | 0.2 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 20 | 0.2 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 18 | 0.2 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 20 | 0.2 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 10 | 0.2 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD11 | 14 | 0.2 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 8 | 0.2 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 17 | 0.2 |
| (2,55) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 1 | 0.2 |
| (1,117) | 1:168:A:ILE:H | 1:122:A:VAL:O | 1 | 0.2 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 11 | 0.2 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 15 | 0.2 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 16 | 0.2 |
| (1,111) | 1:159:A:TYR:H | 1:167:A:LEU:O | 19 | 0.2 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 14 | 0.2 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 6 | 0.2 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 10 | 0.2 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 8 | 0.2 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 14 | 0.2 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 20 | 0.2 |
| (1,92) | 1:133:A:LYS:N | 1:129:A:THR:O | 6 | 0.2 |
| (1,88) | 1:131:A:ALA:N | 1:127:A:ASP:O | 19 | 0.2 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 10 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,77) | 1:112:A:ASP:H | 1:108:A:LEU:O | 14 | 0.2 |
| (1,77) | 1:112:A:ASP:H | 1:108:A:LEU:O | 17 | 0.2 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 6 | 0.2 |
| (1,74) | 1:110:A:LEU:N | 1:106:A:PHE:O | 15 | 0.2 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 5 | 0.2 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 17 | 0.2 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 1 | 0.2 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 6 | 0.2 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 12 | 0.2 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 20 | 0.2 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 1 | 0.2 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 6 | 0.2 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 12 | 0.2 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 13 | 0.2 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 5 | 0.2 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 1 | 0.2 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 3 | 0.2 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 10 | 0.2 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 19 | 0.2 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 20 | 0.2 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 14 | 0.2 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 8 | 0.2 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 14 | 0.2 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 1 | 0.2 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 4 | 0.2 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 14 | 0.2 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 1 | 0.2 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 2 | 0.2 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 3 | 0.2 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 9 | 0.2 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 11 | 0.2 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 13 | 0.2 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 15 | 0.2 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 19 | 0.2 |
| (1,18) | 1:15:A:LEU:N | 1:11:A:LEU:O | 3 | 0.2 |
| (1,18) | 1:15:A:LEU:N | 1:11:A:LEU:O | 20 | 0.2 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 16 | 0.2 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 5 | 0.2 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 8 | 0.2 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 17 | 0.2 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 20 | 0.2 |
| (1,4) | 1:8:A:SER:N | 1:4:A:MET:O | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HG3 | 14 | 0.19 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 1 | 0.19 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 2 | 0.19 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 6 | 0.19 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 17 | 0.19 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 9 | 0.19 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 15 | 0.19 |
| (4,439) | 1:176:A:ILE:HG22 | 1:109:A:ILE:HB | 6 | 0.19 |
| (4,396) | 1:34:A:VAL:HA | 1:34:A:VAL:HG22 | 8 | 0.19 |
| (4,387) | 1:83:A:GLU:HA | 1:82:A:VAL:HG12 | 15 | 0.19 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 15 | 0.19 |
| (4,379) | 1:50:A:MET:HA | 1:39:A:ALA:HB3 | 20 | 0.19 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 5 | 0.19 |
| (4,319) | 1:26:A:LEU:HD23 | 1:14:A:VAL:HA | 9 | 0.19 |
| (4,311) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 2 | 0.19 |
| (4,311) | 1:143:A:VAL:HG12 | 1:178:A:VAL:HA | 11 | 0.19 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 4 | 0.19 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 19 | 0.19 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 5 | 0.19 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 7 | 0.19 |
| (4,227) | 1:8:A:SER:HB3 | 1:65:A:PHE:HE1 | 18 | 0.19 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 17 | 0.19 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 2 | 0.19 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB2 | 11 | 0.19 |
| (4,122) | 1:111:A:LYS:H | 1:109:A:ILE:HG22 | 8 | 0.19 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 16 | 0.19 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 1 | 0.19 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 19 | 0.19 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 11 | 0.19 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 1 | 0.19 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 4 | 0.19 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 15 | 0.19 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 16 | 0.19 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 19 | 0.19 |
| (4,8) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HD1 | 4 | 0.19 |
| (4,3) | 1:65:A:PHE:HD1 | 1:15:A:LEU:HD23 | 10 | 0.19 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 3 | 0.19 |
| (2,3913) | 2:201:A:NAD:H51N | 2:201:A:NAD:H2N | 17 | 0.19 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 18 | 0.19 |
| (2,3841) | 1:76:A:ALA:HB1 | 1:76:A:ALA:H | 5 | 0.19 |
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 9 | 0.19 |
| (2,3841) | 1:76:A:ALA:HB3 | 1:76:A:ALA:H | 10 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3841) | 1:76:A:ALA:HB2 | 1:76:A:ALA:H | 11 | 0.19 |
| (2,3841) | 1:76:A:ALA:HB3 | 1:76:A:ALA:H | 13 | 0.19 |
| (2,3841) | 1:76:A:ALA:HB3 | 1:76:A:ALA:H | 18 | 0.19 |
| (2,3837) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HA | 2 | 0.19 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 7 | 0.19 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 8 | 0.19 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 7 | 0.19 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 9 | 0.19 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 10 | 0.19 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 18 | 0.19 |
| (2,3829) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 13 | 0.19 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 1 | 0.19 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 11 | 0.19 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 13 | 0.19 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 15 | 0.19 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 19 | 0.19 |
| (2,3824) | 1:41:A:MET:HE1 | 1:11:A:LEU:HD12 | 20 | 0.19 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG23 | 11 | 0.19 |
| (2,3821) | 1:144:A:LEU:HD11 | 1:109:A:ILE:HG21 | 13 | 0.19 |
| (2,3819) | 1:151:A:MET:HE2 | 1:171:A:VAL:HG12 | 7 | 0.19 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 14 | 0.19 |
| (2,3816) | 1:22:A:ILE:HG21 | 1:14:A:VAL:HG23 | 18 | 0.19 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 20 | 0.19 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 10 | 0.19 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 19 | 0.19 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 5 | 0.19 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 8 | 0.19 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 18 | 0.19 |
| (2,3777) | 1:86:A:LEU:HD21 | 1:86:A:LEU:HB2 | 10 | 0.19 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 3 | 0.19 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 20 | 0.19 |
| (2,3763) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD11 | 5 | 0.19 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 6 | 0.19 |
| (2,3763) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD12 | 14 | 0.19 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG23 | 3 | 0.19 |
| (2,3710) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 17 | 0.19 |
| (2,3705) | 1:7:A:VAL:HG11 | 1:7:A:VAL:HA | 5 | 0.19 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 16 | 0.19 |
| (2,3705) | 1:7:A:VAL:HG13 | 1:7:A:VAL:HA | 20 | 0.19 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 1 | 0.19 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 3 | 0.19 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 4 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 20 | 0.19 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 4 | 0.19 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 8 | 0.19 |
| (2,3654) | 1:96:A:VAL:HG22 | 1:96:A:VAL:HA | 11 | 0.19 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 13 | 0.19 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 14 | 0.19 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 1 | 0.19 |
| (2,3653) | 1:14:A:VAL:HG21 | 1:19:A:PRO:HA | 14 | 0.19 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 4 | 0.19 |
| (2,3573) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 19 | 0.19 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 1 | 0.19 |
| (2,3564) | 1:108:A:LEU:HB3 | 1:111:A:LYS:HE2 | 10 | 0.19 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 5 | 0.19 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 9 | 0.19 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 10 | 0.19 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 14 | 0.19 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 15 | 0.19 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 18 | 0.19 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 19 | 0.19 |
| (2,3531) | 1:151:A:MET:HE1 | 1:175:A:PHE:HB3 | 9 | 0.19 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 2 | 0.19 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 8 | 0.19 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 15 | 0.19 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 16 | 0.19 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 19 | 0.19 |
| (2,3502) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HA | 16 | 0.19 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 1 | 0.19 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 12 | 0.19 |
| (2,3479) | 1:151:A:MET:HE3 | 1:171:A:VAL:HA | 20 | 0.19 |
| (2,3473) | 1:146:A:VAL:HG23 | 1:96:A:VAL:HA | 4 | 0.19 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 17 | 0.19 |
| (2,3456) | 1:167:A:LEU:HD13 | 1:123:A:HIS:HA | 8 | 0.19 |
| (2,3428) | 1:108:A:LEU:HD11 | 2:201:A:NAD:H2A | 8 | 0.19 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 20 | 0.19 |
| (2,3399) | 1:21:A:LEU:HD13 | 1:21:A:LEU:H | 3 | 0.19 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 14 | 0.19 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 2 | 0.19 |
| (2,3372) | 1:20:A:ALA:HB1 | 1:20:A:ALA:H | 9 | 0.19 |
| (2,3288) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 18 | 0.19 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 7 | 0.19 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 19 | 0.19 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 20 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 7 | 0.19 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 11 | 0.19 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 17 | 0.19 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 18 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 1 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 2 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 3 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 4 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 6 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 7 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 8 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 9 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 10 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 11 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 12 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 13 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 14 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 15 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 16 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 17 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 18 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 19 | 0.19 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 20 | 0.19 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 2 | 0.19 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 4 | 0.19 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 5 | 0.19 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 8 | 0.19 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 3 | 0.19 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 6 | 0.19 |
| (2,3166) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 11 | 0.19 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 12 | 0.19 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 16 | 0.19 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 17 | 0.19 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD23 | 18 | 0.19 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 3 | 0.19 |
| (2,2918) | 1:76:A:ALA:HB3 | 1:78:A:GLN:HE22 | 2 | 0.19 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 18 | 0.19 |
| (2,2748) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 10 | 0.19 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 8 | 0.19 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 19 | 0.19 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 10 | 0.19 |
| (2,2506) | 1:64:A:ARG:H | 1:76:A:ALA:HB3 | 14 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 3 | 0.19 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 7 | 0.19 |
| (2,2417) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 4 | 0.19 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 12 | 0.19 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 19 | 0.19 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 8 | 0.19 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 10 | 0.19 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 15 | 0.19 |
| (2,2189) | 1:81:A:SER:HA | 1:82:A:VAL:H | 15 | 0.19 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 8 | 0.19 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 15 | 0.19 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD23 | 20 | 0.19 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 12 | 0.19 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 11 | 0.19 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 13 | 0.19 |
| (2,1939) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 13 | 0.19 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 3 | 0.19 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 4 | 0.19 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 11 | 0.19 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 13 | 0.19 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD11 | 14 | 0.19 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 19 | 0.19 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 14 | 0.19 |
| (2,1844) | 1:110:A:LEU:HD21 | 1:110:A:LEU:HB3 | 20 | 0.19 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 5 | 0.19 |
| (2,1830) | 1:34:A:VAL:HG13 | 1:50:A:MET:HE2 | 13 | 0.19 |
| (2,1805) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 1 | 0.19 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 4 | 0.19 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 7 | 0.19 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 11 | 0.19 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 13 | 0.19 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 16 | 0.19 |
| (2,1792) | 1:59:A:THR:HG21 | 1:58:A:GLU:HG2 | 1 | 0.19 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 4 | 0.19 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 13 | 0.19 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 1 | 0.19 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 3 | 0.19 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 6 | 0.19 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 8 | 0.19 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 10 | 0.19 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 14 | 0.19 |
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 15 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1747) | 1:14:A:VAL:HB | 1:14:A:VAL:HA | 18 | 0.19 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 2 | 0.19 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 5 | 0.19 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 10 | 0.19 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 14 | 0.19 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 1 | 0.19 |
| (2,1599) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 14 | 0.19 |
| (2,1549) | 1:37:A:LEU:HD13 | 1:41:A:MET:HG2 | 6 | 0.19 |
| (2,1541) | 1:143:A:VAL:HG13 | 1:132:A:ARG:HA | 4 | 0.19 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 1 | 0.19 |
| (2,1524) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 4 | 0.19 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 14 | 0.19 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 2 | 0.19 |
| (2,1474) | 1:110:A:LEU:HD21 | 1:110:A:LEU:H | 4 | 0.19 |
| (2,1468) | 1:22:A:ILE:HG22 | 1:10:A:PHE:HZ | 12 | 0.19 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 1 | 0.19 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 7 | 0.19 |
| (2,1438) | 1:146:A:VAL:HG13 | 1:97:A:LEU:H | 6 | 0.19 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 2 | 0.19 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 16 | 0.19 |
| (2,1432) | 1:38:A:LEU:HD13 | 1:39:A:ALA:H | 7 | 0.19 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 13 | 0.19 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 17 | 0.19 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 13 | 0.19 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 15 | 0.19 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 9 | 0.19 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 11 | 0.19 |
| (2,1301) | 1:34:A:VAL:HG12 | 1:38:A:LEU:H | 10 | 0.19 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 7 | 0.19 |
| (2,1288) | 1:167:A:LEU:HD22 | 1:167:A:LEU:HA | 7 | 0.19 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 9 | 0.19 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 20 | 0.19 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 9 | 0.19 |
| (2,1218) | 1:177:A:LYS:HG2 | 1:177:A:LYS:HA | 9 | 0.19 |
| (2,1218) | 1:177:A:LYS:HG2 | 1:177:A:LYS:HA | 16 | 0.19 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 11 | 0.19 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 20 | 0.19 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 16 | 0.19 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 9 | 0.19 |
| (2,1014) | 1:160:A:LEU:H | 1:89:A:GLU:H | 15 | 0.19 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 1 | 0.19 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 4 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 5 | 0.19 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 10 | 0.19 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 16 | 0.19 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 3 | 0.19 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 6 | 0.19 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 10 | 0.19 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 19 | 0.19 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 13 | 0.19 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 16 | 0.19 |
| (2,726) | 1:20:A:ALA:HB2 | 1:23:A:GLY:H | 12 | 0.19 |
| (2,726) | 1:20:A:ALA:HB2 | 1:23:A:GLY:H | 20 | 0.19 |
| (2,718) | 1:91:A:GLN:HE21 | 1:89:A:GLU:HB2 | 5 | 0.19 |
| (2,718) | 1:91:A:GLN:HE21 | 1:89:A:GLU:HB2 | 17 | 0.19 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 19 | 0.19 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 11 | 0.19 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 15 | 0.19 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 4 | 0.19 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 11 | 0.19 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 3 | 0.19 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 6 | 0.19 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 8 | 0.19 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 11 | 0.19 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 12 | 0.19 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 19 | 0.19 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 6 | 0.19 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 8 | 0.19 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 9 | 0.19 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 10 | 0.19 |
| (2,511) | 1:128:A:ILE:HG21 | 1:129:A:THR:H | 17 | 0.19 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 2 | 0.19 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 9 | 0.19 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 20 | 0.19 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 16 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 1 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 2 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 3 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 8 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 13 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 14 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 15 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 17 | 0.19 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 19 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 13 | 0.19 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 2 | 0.19 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 4 | 0.19 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 7 | 0.19 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 12 | 0.19 |
| (2,268) | 1:14:A:VAL:HG22 | 1:21:A:LEU:H | 5 | 0.19 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 10 | 0.19 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 15 | 0.19 |
| (2,224) | 1:81:A:SER:HA | 1:82:A:VAL:H | 20 | 0.19 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 13 | 0.19 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 14 | 0.19 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 19 | 0.19 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 20 | 0.19 |
| (2,137) | 1:103:A:GLU:H | 1:140:A:LYS:HB2 | 10 | 0.19 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 6 | 0.19 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 16 | 0.19 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 3 | 0.19 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 12 | 0.19 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 15 | 0.19 |
| (2,61) | 1:166:A:TRP:HE1 | 1:126:A:GLN:HB2 | 6 | 0.19 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 17 | 0.19 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 7 | 0.19 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 20 | 0.19 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 14 | 0.19 |
| (2,13) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 18 | 0.19 |
| (2,2) | 1:159:A:TYR:HD1 | 1:94:A:PRO:HB3 | 20 | 0.19 |
| (1,117) | 1:168:A:ILE:H | 1:122:A:VAL:O | 19 | 0.19 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 9 | 0.19 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 20 | 0.19 |
| (1,111) | 1:159:A:TYR:H | 1:167:A:LEU:O | 9 | 0.19 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 2 | 0.19 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 16 | 0.19 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 4 | 0.19 |
| (1,92) | 1:133:A:LYS:N | 1:129:A:THR:O | 9 | 0.19 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 13 | 0.19 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 7 | 0.19 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 16 | 0.19 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 15 | 0.19 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 18 | 0.19 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 2 | 0.19 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 2 | 0.19 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 8 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 10 | 0.19 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 11 | 0.19 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 13 | 0.19 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 13 | 0.19 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 9 | 0.19 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 16 | 0.19 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 6 | 0.19 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 14 | 0.19 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 20 | 0.19 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 11 | 0.19 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 16 | 0.19 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 7 | 0.19 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 17 | 0.19 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 6 | 0.19 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 9 | 0.19 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 6 | 0.19 |
| (1,2) | 1:7:A:VAL:N | 1:3:A:HIS:O | 7 | 0.19 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 9 | 0.18 |
| (4,443) | 1:48:A:ILE:HD13 | 1:38:A:LEU:HB2 | 20 | 0.18 |
| (4,442) | 1:178:A:VAL:HG21 | 1:144:A:LEU:HG | 3 | 0.18 |
| (4,350) | 1:6:A:LYS:HE2 | 1:44:A:LYS:HG3 | 8 | 0.18 |
| (4,325) | 1:7:A:VAL:HG13 | 1:10:A:PHE:HB3 | 4 | 0.18 |
| (4,319) | 1:26:A:LEU:HD23 | 1:14:A:VAL:HA | 11 | 0.18 |
| (4,307) | 1:26:A:LEU:HD21 | 1:15:A:LEU:HA | 12 | 0.18 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 5 | 0.18 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 2 | 0.18 |
| (4,234) | 1:53:A:LEU:HA | 1:53:A:LEU:H | 18 | 0.18 |
| (4,208) | 1:14:A:VAL:HG22 | 1:11:A:LEU:HA | 11 | 0.18 |
| (4,174) | 1:97:A:LEU:H | 1:152:A:ALA:H | 12 | 0.18 |
| (4,61) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 1 | 0.18 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 17 | 0.18 |
| (4,8) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HD1 | 13 | 0.18 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 7 | 0.18 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 14 | 0.18 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 4 | 0.18 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 1 | 0.18 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 15 | 0.18 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 18 | 0.18 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 5 | 0.18 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 14 | 0.18 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 17 | 0.18 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 16 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3841) | 1:76:A:ALA:HB3 | 1:76:A:ALA:H | 7 | 0.18 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 10 | 0.18 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 1 | 0.18 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 3 | 0.18 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 6 | 0.18 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD12 | 12 | 0.18 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 14 | 0.18 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 15 | 0.18 |
| (2,3829) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 7 | 0.18 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 1 | 0.18 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 3 | 0.18 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 4 | 0.18 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD11 | 14 | 0.18 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 20 | 0.18 |
| (2,3819) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 5 | 0.18 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 19 | 0.18 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 16 | 0.18 |
| (2,3809) | 1:176:A:ILE:HB | 1:110:A:LEU:HD11 | 5 | 0.18 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 2 | 0.18 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 10 | 0.18 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 14 | 0.18 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 15 | 0.18 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 16 | 0.18 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 17 | 0.18 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 4 | 0.18 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 13 | 0.18 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 19 | 0.18 |
| (2,3791) | 1:142:A:VAL:HG23 | 1:143:A:VAL:HB | 10 | 0.18 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 9 | 0.18 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 11 | 0.18 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 16 | 0.18 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 19 | 0.18 |
| (2,3772) | 1:151:A:MET:HE1 | 1:174:A:GLU:HG2 | 19 | 0.18 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD12 | 12 | 0.18 |
| (2,3759) | 1:53:A:LEU:HD11 | 1:53:A:LEU:HB2 | 15 | 0.18 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 10 | 0.18 |
| (2,3710) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HA | 14 | 0.18 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 17 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 3 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 6 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG22 | 1:96:A:VAL:HA | 7 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 10 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 12 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 16 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 19 | 0.18 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 20 | 0.18 |
| (2,3653) | 1:14:A:VAL:HG22 | 1:19:A:PRO:HA | 17 | 0.18 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 20 | 0.18 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 2 | 0.18 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE2 | 10 | 0.18 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 15 | 0.18 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE3 | 17 | 0.18 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 8 | 0.18 |
| (2,3503) | 1:34:A:VAL:HG13 | 1:34:A:VAL:HA | 1 | 0.18 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 5 | 0.18 |
| (2,3503) | 1:34:A:VAL:HG13 | 1:34:A:VAL:HA | 18 | 0.18 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 20 | 0.18 |
| (2,3495) | 1:82:A:VAL:HG11 | 1:82:A:VAL:HA | 4 | 0.18 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 14 | 0.18 |
| (2,3490) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HA | 14 | 0.18 |
| (2,3484) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 19 | 0.18 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 12 | 0.18 |
| (2,3470) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 19 | 0.18 |
| (2,3430) | 1:128:A:ILE:HD11 | 1:127:A:ASP:H | 15 | 0.18 |
| (2,3428) | 1:108:A:LEU:HD12 | 2:201:A:NAD:H2A | 20 | 0.18 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 2 | 0.18 |
| (2,3424) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 13 | 0.18 |
| (2,3424) | 1:165:A:VAL:HG23 | 2:201:A:NAD:H5N | 18 | 0.18 |
| (2,3409) | 1:84:A:VAL:HG11 | 1:85:A:ASP:H | 10 | 0.18 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 2 | 0.18 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 3 | 0.18 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 5 | 0.18 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 8 | 0.18 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 15 | 0.18 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 16 | 0.18 |
| (2,3382) | 1:53:A:LEU:HD11 | 1:67:A:PHE:HZ | 18 | 0.18 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 3 | 0.18 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 1 | 0.18 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 8 | 0.18 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 9 | 0.18 |
| (2,3174) | 1:24:A:LEU:HD11 | 1:32:A:ALA:HB2 | 16 | 0.18 |
| (2,3168) | 1:176:A:ILE:HB | 1:176:A:ILE:HG12 | 5 | 0.18 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 3 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 2 | 0.18 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 7 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 3 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 7 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 10 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD23 | 13 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD22 | 15 | 0.18 |
| (2,3127) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD22 | 20 | 0.18 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD21 | 2 | 0.18 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 20 | 0.18 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 10 | 0.18 |
| (2,2657) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 18 | 0.18 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 2 | 0.18 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 10 | 0.18 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 16 | 0.18 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 19 | 0.18 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 20 | 0.18 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 10 | 0.18 |
| (2,2417) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 2 | 0.18 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 4 | 0.18 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 5 | 0.18 |
| (2,2367) | 1:48:A:ILE:HG23 | 1:48:A:ILE:H | 4 | 0.18 |
| (2,2367) | 1:48:A:ILE:HG23 | 1:48:A:ILE:H | 7 | 0.18 |
| (2,2367) | 1:48:A:ILE:HG22 | 1:48:A:ILE:H | 15 | 0.18 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 20 | 0.18 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 9 | 0.18 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 10 | 0.18 |
| (2,2232) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 7 | 0.18 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 6 | 0.18 |
| (2,2189) | 1:81:A:SER:HA | 1:82:A:VAL:H | 20 | 0.18 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 10 | 0.18 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 8 | 0.18 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 1 | 0.18 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 6 | 0.18 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 11 | 0.18 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD11 | 14 | 0.18 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 20 | 0.18 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 11 | 0.18 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 8 | 0.18 |
| (2,2041) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 14 | 0.18 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 4 | 0.18 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 6 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 4 | 0.18 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 7 | 0.18 |
| (2,1958) | 1:168:A:ILE:HD11 | 1:158:A:PHE:HE1 | 11 | 0.18 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 8 | 0.18 |
| (2,1871) | 1:97:A:LEU:HD21 | 1:151:A:MET:HG3 | 9 | 0.18 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 2 | 0.18 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 15 | 0.18 |
| (2,1860) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 10 | 0.18 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 7 | 0.18 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 10 | 0.18 |
| (2,1810) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 5 | 0.18 |
| (2,1810) | 1:21:A:LEU:HD12 | 1:21:A:LEU:HB3 | 20 | 0.18 |
| (2,1800) | 1:53:A:LEU:HD12 | 1:37:A:LEU:HG | 17 | 0.18 |
| (2,1796) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 20 | 0.18 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 4 | 0.18 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 15 | 0.18 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 7 | 0.18 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 18 | 0.18 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 19 | 0.18 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 4 | 0.18 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 15 | 0.18 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 8 | 0.18 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 14 | 0.18 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 17 | 0.18 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 20 | 0.18 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 4 | 0.18 |
| (2,1474) | 1:110:A:LEU:HD23 | 1:110:A:LEU:H | 1 | 0.18 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 8 | 0.18 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 20 | 0.18 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 20 | 0.18 |
| (2,1435) | 1:15:A:LEU:HD21 | 1:15:A:LEU:H | 9 | 0.18 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 1 | 0.18 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 14 | 0.18 |
| (2,1407) | 1:95:A:ALA:HB2 | 1:95:A:ALA:H | 5 | 0.18 |
| (2,1403) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 9 | 0.18 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 2 | 0.18 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 3 | 0.18 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 4 | 0.18 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 8 | 0.18 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 16 | 0.18 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 8 | 0.18 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 7 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 13 | 0.18 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 14 | 0.18 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 19 | 0.18 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 18 | 0.18 |
| (2,1131) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 11 | 0.18 |
| (2,1110) | 1:76:A:ALA:H | 1:75:A:ARG:H | 2 | 0.18 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 20 | 0.18 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 1 | 0.18 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 2 | 0.18 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 3 | 0.18 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 7 | 0.18 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 11 | 0.18 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 14 | 0.18 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 18 | 0.18 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 10 | 0.18 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 16 | 0.18 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 18 | 0.18 |
| (2,815) | 1:102:A:ALA:H | 1:101:A:THR:HG23 | 9 | 0.18 |
| (2,726) | 1:20:A:ALA:HB2 | 1:23:A:GLY:H | 11 | 0.18 |
| (2,718) | 1:91:A:GLN:HE21 | 1:89:A:GLU:HB2 | 19 | 0.18 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 20 | 0.18 |
| (2,673) | 1:70:A:ASN:HD22 | 1:50:A:MET:HG3 | 3 | 0.18 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 1 | 0.18 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 7 | 0.18 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 9 | 0.18 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 12 | 0.18 |
| (2,550) | 1:105:A:ASN:H | 1:102:A:ALA:HB3 | 15 | 0.18 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 14 | 0.18 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 1 | 0.18 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 15 | 0.18 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 11 | 0.18 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 10 | 0.18 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 14 | 0.18 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG11 | 18 | 0.18 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 10 | 0.18 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 6 | 0.18 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 9 | 0.18 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 10 | 0.18 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 14 | 0.18 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 16 | 0.18 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 1 | 0.18 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 18 | 0.18 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 18 | 0.18 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 2 | 0.18 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 14 | 0.18 |
| (2,190) | 1:13:A:LEU:H | 1:13:A:LEU:HB3 | 5 | 0.18 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 12 | 0.18 |
| (2,181) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 15 | 0.18 |
| (2,168) | 1:39:A:ALA:H | 1:41:A:MET:H | 12 | 0.18 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 2 | 0.18 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 4 | 0.18 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 15 | 0.18 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 16 | 0.18 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 14 | 0.18 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 11 | 0.18 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 18 | 0.18 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 2 | 0.18 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 12 | 0.18 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 3 | 0.18 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 6 | 0.18 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 14 | 0.18 |
| (1,111) | 1:159:A:TYR:H | 1:167:A:LEU:O | 10 | 0.18 |
| (1,111) | 1:159:A:TYR:H | 1:167:A:LEU:O | 11 | 0.18 |
| (1,108) | 1:151:A:MET:N | 1:148:A:ALA:O | 5 | 0.18 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 15 | 0.18 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 14 | 0.18 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 3 | 0.18 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 11 | 0.18 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 10 | 0.18 |
| (1,94) | 1:134:A:VAL:N | 1:130:A:THR:O | 3 | 0.18 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 19 | 0.18 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 11 | 0.18 |
| (1,83) | 1:122:A:VAL:H | 1:168:A:ILE:O | 17 | 0.18 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 1 | 0.18 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 8 | 0.18 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 3 | 0.18 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 1 | 0.18 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 3 | 0.18 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 8 | 0.18 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 20 | 0.18 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 15 | 0.18 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 17 | 0.18 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 11 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 14 | 0.18 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 3 | 0.18 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 8 | 0.18 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 10 | 0.18 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 11 | 0.18 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 12 | 0.18 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 13 | 0.18 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 9 | 0.18 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 5 | 0.18 |
| (1,24) | 1:37:A:LEU:N | 1:33:A:PRO:O | 4 | 0.18 |
| (1,24) | 1:37:A:LEU:N | 1:33:A:PRO:O | 16 | 0.18 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 16 | 0.18 |
| (1,17) | 1:15:A:LEU:H | 1:11:A:LEU:O | 3 | 0.18 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 18 | 0.18 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 2 | 0.18 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 7 | 0.18 |
| (4,453) | 1:48:A:ILE:HG13 | 1:38:A:LEU:HA | 2 | 0.17 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 15 | 0.17 |
| (4,448) | 1:110:A:LEU:HD22 | 1:144:A:LEU:HG | 14 | 0.17 |
| (4,440) | 1:15:A:LEU:HD22 | 1:74:A:ILE:HB | 14 | 0.17 |
| (4,409) | 1:4:A:MET:HE1 | 1:59:A:THR:HG23 | 2 | 0.17 |
| (4,379) | 1:50:A:MET:HA | 1:35:A:LYS:HG2 | 13 | 0.17 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 11 | 0.17 |
| (4,325) | 1:7:A:VAL:HG13 | 1:10:A:PHE:HB3 | 18 | 0.17 |
| (4,320) | 1:151:A:MET:HE2 | 1:158:A:PHE:HB2 | 9 | 0.17 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 12 | 0.17 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 20 | 0.17 |
| (4,198) | 1:176:A:ILE:HD11 | 1:106:A:PHE:HE1 | 3 | 0.17 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 7 | 0.17 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 15 | 0.17 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 16 | 0.17 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 17 | 0.17 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD12 | 5 | 0.17 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 19 | 0.17 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 3 | 0.17 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 13 | 0.17 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 6 | 0.17 |
| (2,3940) | 1:134:A:VAL:HG11 | 2:201:A:NAD:H2N | 10 | 0.17 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 11 | 0.17 |
| (2,3920) | 1:115:A:LYS:H | 2:201:A:NAD:H8A | 6 | 0.17 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 7 | 0.17 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 10 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 13 | 0.17 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 15 | 0.17 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 19 | 0.17 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 2 | 0.17 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 5 | 0.17 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 9 | 0.17 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 14 | 0.17 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 18 | 0.17 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 15 | 0.17 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 18 | 0.17 |
| (2,3836) | 1:168:A:ILE:HD12 | 1:171:A:VAL:HG11 | 12 | 0.17 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 16 | 0.17 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD12 | 5 | 0.17 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 16 | 0.17 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 20 | 0.17 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 8 | 0.17 |
| (2,3824) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD11 | 10 | 0.17 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 9 | 0.17 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 17 | 0.17 |
| (2,3819) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 1 | 0.17 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 8 | 0.17 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 20 | 0.17 |
| (2,3814) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 1 | 0.17 |
| (2,3813) | 1:56:A:ILE:HD12 | 1:11:A:LEU:HD13 | 5 | 0.17 |
| (2,3804) | 1:128:A:ILE:HG23 | 1:129:A:THR:HG21 | 10 | 0.17 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 6 | 0.17 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 6 | 0.17 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 7 | 0.17 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 8 | 0.17 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 9 | 0.17 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 18 | 0.17 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 19 | 0.17 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 9 | 0.17 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 11 | 0.17 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 12 | 0.17 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 20 | 0.17 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 5 | 0.17 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 8 | 0.17 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 12 | 0.17 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 17 | 0.17 |
| (2,3763) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD11 | 15 | 0.17 |
| (2,3761) | 1:117:A:MET:HE1 | 1:117:A:MET:HB2 | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 8 | 0.17 |
| (2,3744) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 2 | 0.17 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 15 | 0.17 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 19 | 0.17 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 10 | 0.17 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 1 | 0.17 |
| (2,3654) | 1:96:A:VAL:HG22 | 1:96:A:VAL:HA | 2 | 0.17 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 17 | 0.17 |
| (2,3654) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 18 | 0.17 |
| (2,3575) | 1:50:A:MET:HE1 | 1:50:A:MET:HG3 | 13 | 0.17 |
| (2,3575) | 1:50:A:MET:HE2 | 1:50:A:MET:HG3 | 17 | 0.17 |
| (2,3565) | 1:71:A:PHE:HB2 | 1:50:A:MET:HE1 | 18 | 0.17 |
| (2,3559) | 1:102:A:ALA:HB1 | 2:201:A:NAD:H4B | 7 | 0.17 |
| (2,3547) | 1:22:A:ILE:HG21 | 1:22:A:ILE:HA | 16 | 0.17 |
| (2,3518) | 1:128:A:ILE:HD12 | 1:128:A:ILE:HA | 13 | 0.17 |
| (2,3518) | 1:128:A:ILE:HD12 | 1:128:A:ILE:HA | 17 | 0.17 |
| (2,3509) | 1:13:A:LEU:HD23 | 1:17:A:HIS:HB2 | 2 | 0.17 |
| (2,3509) | 1:13:A:LEU:HD21 | 1:17:A:HIS:HB2 | 14 | 0.17 |
| (2,3503) | 1:34:A:VAL:HG11 | 1:34:A:VAL:HA | 14 | 0.17 |
| (2,3473) | 1:146:A:VAL:HG23 | 1:96:A:VAL:HA | 8 | 0.17 |
| (2,3409) | 1:84:A:VAL:HG13 | 1:85:A:ASP:H | 18 | 0.17 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 1 | 0.17 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 20 | 0.17 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 12 | 0.17 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 20 | 0.17 |
| (2,3355) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 17 | 0.17 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 2 | 0.17 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 17 | 0.17 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 1 | 0.17 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 2 | 0.17 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 4 | 0.17 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 17 | 0.17 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 9 | 0.17 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 10 | 0.17 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 12 | 0.17 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 15 | 0.17 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 17 | 0.17 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD22 | 1 | 0.17 |
| (2,3127) | 1:97:A:LEU:HD12 | 1:124:A:LEU:HD22 | 6 | 0.17 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 8 | 0.17 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 16 | 0.17 |
| (2,2925) | 1:57:A:VAL:H | 1:53:A:LEU:HD23 | 14 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2657) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 11 | 0.17 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 2 | 0.17 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 3 | 0.17 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 13 | 0.17 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 1 | 0.17 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 6 | 0.17 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 13 | 0.17 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 14 | 0.17 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 15 | 0.17 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 1 | 0.17 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 3 | 0.17 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 14 | 0.17 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 3 | 0.17 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 11 | 0.17 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 9 | 0.17 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 18 | 0.17 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 13 | 0.17 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 11 | 0.17 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG12 | 14 | 0.17 |
| (2,2232) | 1:21:A:LEU:H | 1:24:A:LEU:HD23 | 11 | 0.17 |
| (2,2210) | 1:48:A:ILE:HD12 | 1:53:A:LEU:H | 8 | 0.17 |
| (2,2192) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 15 | 0.17 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 2 | 0.17 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 12 | 0.17 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD23 | 13 | 0.17 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 16 | 0.17 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 17 | 0.17 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 1 | 0.17 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 2 | 0.17 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 14 | 0.17 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 17 | 0.17 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 16 | 0.17 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 5 | 0.17 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 1 | 0.17 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 2 | 0.17 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 6 | 0.17 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 13 | 0.17 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 20 | 0.17 |
| (2,1889) | 1:4:A:MET:HE1 | 1:4:A:MET:HA | 6 | 0.17 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 19 | 0.17 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD12 | 8 | 0.17 |
| (2,1861) | 1:41:A:MET:HE3 | 1:11:A:LEU:HD11 | 10 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 11 | 0.17 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 17 | 0.17 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 11 | 0.17 |
| (2,1828) | 1:151:A:MET:HE2 | 1:151:A:MET:HG3 | 5 | 0.17 |
| (2,1807) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 4 | 0.17 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 3 | 0.17 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 20 | 0.17 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 2 | 0.17 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 12 | 0.17 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 18 | 0.17 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 6 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 2 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 3 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 4 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 11 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 12 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 13 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 15 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 16 | 0.17 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 19 | 0.17 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 7 | 0.17 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 1 | 0.17 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 8 | 0.17 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 20 | 0.17 |
| (2,1622) | 1:73:A:LYS:HE3 | 1:25:A:ASP:HA | 17 | 0.17 |
| (2,1563) | 1:48:A:ILE:HG23 | 1:53:A:LEU:HB2 | 16 | 0.17 |
| (2,1555) | 1:84:A:VAL:HG22 | 1:85:A:ASP:HB2 | 1 | 0.17 |
| (2,1541) | 1:143:A:VAL:HG11 | 1:132:A:ARG:HA | 18 | 0.17 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 20 | 0.17 |
| (2,1513) | 1:26:A:LEU:HD13 | 1:32:A:ALA:HA | 13 | 0.17 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 5 | 0.17 |
| (2,1509) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 16 | 0.17 |
| (2,1509) | 1:151:A:MET:HE3 | 1:171:A:VAL:HA | 19 | 0.17 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 13 | 0.17 |
| (2,1455) | 1:165:A:VAL:HG23 | 2:201:A:NAD:H5N | 18 | 0.17 |
| (2,1432) | 1:38:A:LEU:HD12 | 1:39:A:ALA:H | 13 | 0.17 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 6 | 0.17 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 1 | 0.17 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 1 | 0.17 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 14 | 0.17 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 8 | 0.17 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 10 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 16 | 0.17 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 10 | 0.17 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 14 | 0.17 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 6 | 0.17 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 7 | 0.17 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 11 | 0.17 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 12 | 0.17 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 13 | 0.17 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 14 | 0.17 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 12 | 0.17 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 13 | 0.17 |
| (2,1164) | 1:131:A:ALA:HB1 | 1:132:A:ARG:H | 17 | 0.17 |
| (2,1155) | 1:86:A:LEU:HD11 | 1:88:A:TYR:HE1 | 5 | 0.17 |
| (2,1075) | 1:56:A:ILE:H | 1:58:A:GLU:H | 5 | 0.17 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 6 | 0.17 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 12 | 0.17 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 13 | 0.17 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 19 | 0.17 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 1 | 0.17 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 8 | 0.17 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 14 | 0.17 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 5 | 0.17 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 12 | 0.17 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 10 | 0.17 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 18 | 0.17 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 11 | 0.17 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD12 | 9 | 0.17 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 8 | 0.17 |
| (2,768) | 1:30:A:GLY:H | 1:26:A:LEU:HD22 | 20 | 0.17 |
| (2,726) | 1:20:A:ALA:HB2 | 1:23:A:GLY:H | 10 | 0.17 |
| (2,708) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 16 | 0.17 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 5 | 0.17 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 5 | 0.17 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 7 | 0.17 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 19 | 0.17 |
| (2,577) | 1:96:A:VAL:H | 1:148:A:ALA:HB2 | 1 | 0.17 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 8 | 0.17 |
| (2,518) | 1:111:A:LYS:HB3 | 1:112:A:ASP:H | 8 | 0.17 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 5 | 0.17 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 3 | 0.17 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 13 | 0.17 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 5 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 3 | 0.17 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 7 | 0.17 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 2 | 0.17 |
| (2,369) | 1:57:A:VAL:HA | 1:57:A:VAL:H | 8 | 0.17 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 2 | 0.17 |
| (2,309) | 1:74:A:ILE:H | 1:73:A:LYS:HG2 | 19 | 0.17 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 10 | 0.17 |
| (2,184) | 1:26:A:LEU:H | 1:19:A:PRO:HA | 19 | 0.17 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 9 | 0.17 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 13 | 0.17 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 3 | 0.17 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 9 | 0.17 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 10 | 0.17 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 12 | 0.17 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 14 | 0.17 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 18 | 0.17 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 8 | 0.17 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 8 | 0.17 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 7 | 0.17 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 9 | 0.17 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 13 | 0.17 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 18 | 0.17 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 13 | 0.17 |
| (2,85) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 19 | 0.17 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 8 | 0.17 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 9 | 0.17 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 5 | 0.17 |
| (2,16) | 1:21:A:LEU:HD12 | 1:10:A:PHE:HE1 | 16 | 0.17 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 16 | 0.17 |
| (2,7) | 1:168:A:ILE:HD11 | 1:158:A:PHE:HE1 | 11 | 0.17 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 14 | 0.17 |
| (1,119) | 1:171:A:VAL:H | 1:114:A:ILE:O | 16 | 0.17 |
| (1,116) | 1:167:A:LEU:N | 1:159:A:TYR:O | 18 | 0.17 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 1 | 0.17 |
| (1,111) | 1:159:A:TYR:H | 1:167:A:LEU:O | 15 | 0.17 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 12 | 0.17 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 5 | 0.17 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 6 | 0.17 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 6 | 0.17 |
| (1,92) | 1:133:A:LYS:N | 1:129:A:THR:O | 7 | 0.17 |
| (1,89) | 1:132:A:ARG:H | 1:128:A:ILE:O | 10 | 0.17 |
| (1,87) | 1:131:A:ALA:H | 1:127:A:ASP:O | 19 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 9 | 0.17 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 10 | 0.17 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 4 | 0.17 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 7 | 0.17 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 20 | 0.17 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 3 | 0.17 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 11 | 0.17 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 6 | 0.17 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 15 | 0.17 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 19 | 0.17 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 4 | 0.17 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 7 | 0.17 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 15 | 0.17 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 19 | 0.17 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 1 | 0.17 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 9 | 0.17 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 16 | 0.17 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 14 | 0.17 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 4 | 0.17 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 18 | 0.17 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 10 | 0.17 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 18 | 0.17 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 14 | 0.17 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 4 | 0.17 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 3 | 0.17 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 12 | 0.17 |
| (1,4) | 1:8:A:SER:N | 1:4:A:MET:O | 6 | 0.17 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 12 | 0.16 |
| (4,442) | 1:178:A:VAL:HG21 | 1:144:A:LEU:HG | 2 | 0.16 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 1 | 0.16 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 5 | 0.16 |
| (4,439) | 1:176:A:ILE:HG21 | 1:177:A:LYS:HG2 | 12 | 0.16 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 16 | 0.16 |
| (4,325) | 1:7:A:VAL:HG11 | 1:10:A:PHE:HB3 | 7 | 0.16 |
| (4,290) | 1:53:A:LEU:HD22 | 1:56:A:ILE:H | 6 | 0.16 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 7 | 0.16 |
| (4,290) | 1:53:A:LEU:HD22 | 1:56:A:ILE:H | 16 | 0.16 |
| (4,259) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 5 | 0.16 |
| (4,227) | 1:8:A:SER:HB3 | 1:65:A:PHE:HE1 | 2 | 0.16 |
| (4,209) | 1:76:A:ALA:HB1 | 1:16:A:ARG:H | 15 | 0.16 |
| (4,95) | 1:41:A:MET:HG3 | 1:51:A:GLU:H | 16 | 0.16 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 7 | 0.16 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 1 | 0.16 |
| (4,8) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HD1 | 15 | 0.16 |
| (2,3959) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H5N | 5 | 0.16 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 3 | 0.16 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 18 | 0.16 |
| (2,3900) | 2:201:A:NAD:H5N | 2:201:A:NAD:H6N | 12 | 0.16 |
| (2,3896) | 2:201:A:NAD:H3D | 2:201:A:NAD:H2N | 15 | 0.16 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 6 | 0.16 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 8 | 0.16 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 9 | 0.16 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 11 | 0.16 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 16 | 0.16 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 20 | 0.16 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 6 | 0.16 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 8 | 0.16 |
| (2,3836) | 1:168:A:ILE:HD13 | 1:171:A:VAL:HG11 | 15 | 0.16 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD13 | 19 | 0.16 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD13 | 8 | 0.16 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 18 | 0.16 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD11 | 3 | 0.16 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 3 | 0.16 |
| (2,3802) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 15 | 0.16 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 16 | 0.16 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 17 | 0.16 |
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 15 | 0.16 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 4 | 0.16 |
| (2,3794) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 11 | 0.16 |
| (2,3794) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 12 | 0.16 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 7 | 0.16 |
| (2,3793) | 1:53:A:LEU:HD22 | 1:56:A:ILE:HB | 16 | 0.16 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 16 | 0.16 |
| (2,3773) | 1:34:A:VAL:HG13 | 1:37:A:LEU:HB3 | 1 | 0.16 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 14 | 0.16 |
| (2,3770) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 4 | 0.16 |
| (2,3770) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 6 | 0.16 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 15 | 0.16 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 18 | 0.16 |
| (2,3763) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD11 | 1 | 0.16 |
| (2,3763) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD12 | 13 | 0.16 |
| (2,3763) | 1:76:A:ALA:HB2 | 1:15:A:LEU:HD11 | 17 | 0.16 |
| (2,3757) | 1:144:A:LEU:HG | 1:101:A:THR:HG22 | 19 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 6 | 0.16 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 10 | 0.16 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 17 | 0.16 |
| (2,3654) | 1:96:A:VAL:HG22 | 1:96:A:VAL:HA | 15 | 0.16 |
| (2,3575) | 1:50:A:MET:HE2 | 1:50:A:MET:HG3 | 7 | 0.16 |
| (2,3575) | 1:50:A:MET:HE2 | 1:50:A:MET:HG3 | 15 | 0.16 |
| (2,3547) | 1:22:A:ILE:HG22 | 1:22:A:ILE:HA | 17 | 0.16 |
| (2,3509) | 1:13:A:LEU:HD22 | 1:17:A:HIS:HB2 | 8 | 0.16 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 2 | 0.16 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 20 | 0.16 |
| (2,3484) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 4 | 0.16 |
| (2,3479) | 1:151:A:MET:HE3 | 1:171:A:VAL:HA | 14 | 0.16 |
| (2,3445) | 1:97:A:LEU:HD23 | 1:166:A:TRP:HE3 | 10 | 0.16 |
| (2,3434) | 1:15:A:LEU:HD12 | 1:65:A:PHE:HE1 | 13 | 0.16 |
| (2,3424) | 1:165:A:VAL:HG23 | 2:201:A:NAD:H5N | 15 | 0.16 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 15 | 0.16 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 11 | 0.16 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 12 | 0.16 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 19 | 0.16 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 4 | 0.16 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 11 | 0.16 |
| (2,3378) | 1:66:A:ALA:HB2 | 1:31:A:TRP:HZ3 | 15 | 0.16 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 5 | 0.16 |
| (2,3345) | 1:41:A:MET:HE1 | 1:10:A:PHE:HE1 | 11 | 0.16 |
| (2,3288) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 17 | 0.16 |
| (2,3288) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 19 | 0.16 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 14 | 0.16 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 19 | 0.16 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 11 | 0.16 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 20 | 0.16 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 11 | 0.16 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD22 | 5 | 0.16 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD21 | 9 | 0.16 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD23 | 12 | 0.16 |
| (2,2982) | 1:160:A:LEU:H | 1:89:A:GLU:H | 13 | 0.16 |
| (2,2852) | 1:85:A:ASP:H | 1:86:A:LEU:H | 13 | 0.16 |
| (2,2657) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 15 | 0.16 |
| (2,2657) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 17 | 0.16 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 7 | 0.16 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 7 | 0.16 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 11 | 0.16 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 18 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 20 | 0.16 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 11 | 0.16 |
| (2,2520) | 1:8:A:SER:H | 1:6:A:LYS:HA | 4 | 0.16 |
| (2,2417) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 3 | 0.16 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 2 | 0.16 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 14 | 0.16 |
| (2,2367) | 1:48:A:ILE:HG23 | 1:48:A:ILE:H | 3 | 0.16 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 11 | 0.16 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 13 | 0.16 |
| (2,2234) | 1:14:A:VAL:HG22 | 1:21:A:LEU:H | 5 | 0.16 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 19 | 0.16 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 19 | 0.16 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 17 | 0.16 |
| (2,2103) | 1:84:A:VAL:HA | 1:85:A:ASP:H | 3 | 0.16 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 7 | 0.16 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 5 | 0.16 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 2 | 0.16 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 4 | 0.16 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 6 | 0.16 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 10 | 0.16 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 19 | 0.16 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 10 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 3 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD13 | 1:106:A:PHE:HE1 | 5 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 10 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD13 | 1:106:A:PHE:HE1 | 14 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD12 | 1:106:A:PHE:HE1 | 15 | 0.16 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 18 | 0.16 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 11 | 0.16 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 14 | 0.16 |
| (2,1932) | 2:201:A:NAD:H3D | 2:201:A:NAD:H2N | 15 | 0.16 |
| (2,1889) | 1:4:A:MET:HE1 | 1:4:A:MET:HA | 12 | 0.16 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 12 | 0.16 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 17 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 5 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 8 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 9 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 11 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 12 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 16 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 17 | 0.16 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 19 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 10 | 0.16 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 9 | 0.16 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 19 | 0.16 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 20 | 0.16 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 8 | 0.16 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 9 | 0.16 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 11 | 0.16 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 15 | 0.16 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 16 | 0.16 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 6 | 0.16 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 7 | 0.16 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 9 | 0.16 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 10 | 0.16 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 18 | 0.16 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 11 | 0.16 |
| (2,1723) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 12 | 0.16 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 18 | 0.16 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE1 | 7 | 0.16 |
| (2,1591) | 1:95:A:ALA:HB1 | 1:149:A:LYS:HA | 6 | 0.16 |
| (2,1588) | 1:152:A:ALA:HB2 | 1:149:A:LYS:HA | 5 | 0.16 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 1 | 0.16 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 2 | 0.16 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 3 | 0.16 |
| (2,1524) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 8 | 0.16 |
| (2,1514) | 1:124:A:LEU:HD13 | 1:167:A:LEU:HA | 19 | 0.16 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 7 | 0.16 |
| (2,1509) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 12 | 0.16 |
| (2,1490) | 1:167:A:LEU:HD13 | 1:166:A:TRP:HA | 12 | 0.16 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 5 | 0.16 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 14 | 0.16 |
| (2,1474) | 1:110:A:LEU:HD21 | 1:110:A:LEU:H | 16 | 0.16 |
| (2,1455) | 1:165:A:VAL:HG22 | 2:201:A:NAD:H5N | 2 | 0.16 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 19 | 0.16 |
| (2,1388) | 1:41:A:MET:HE1 | 1:41:A:MET:H | 9 | 0.16 |
| (2,1378) | 1:50:A:MET:HE2 | 1:67:A:PHE:HZ | 6 | 0.16 |
| (2,1339) | 1:54:A:LYS:HA | 1:67:A:PHE:HE1 | 20 | 0.16 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 2 | 0.16 |
| (2,1321) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 17 | 0.16 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 14 | 0.16 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 17 | 0.16 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 11 | 0.16 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 17 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 18 | 0.16 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 1 | 0.16 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 17 | 0.16 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 18 | 0.16 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 6 | 0.16 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 18 | 0.16 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 4 | 0.16 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 2 | 0.16 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 3 | 0.16 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 9 | 0.16 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 10 | 0.16 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 13 | 0.16 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 20 | 0.16 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 1 | 0.16 |
| (2,1110) | 1:76:A:ALA:H | 1:75:A:ARG:H | 19 | 0.16 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 5 | 0.16 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 19 | 0.16 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 16 | 0.16 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 8 | 0.16 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 9 | 0.16 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 20 | 0.16 |
| (2,996) | 1:164:A:GLY:H | 1:91:A:GLN:HE22 | 5 | 0.16 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 18 | 0.16 |
| (2,862) | 1:76:A:ALA:H | 1:74:A:ILE:HD11 | 9 | 0.16 |
| (2,822) | 1:148:A:ALA:H | 1:96:A:VAL:HB | 5 | 0.16 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 19 | 0.16 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD11 | 15 | 0.16 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 1 | 0.16 |
| (2,772) | 1:86:A:LEU:HG | 1:87:A:GLY:H | 12 | 0.16 |
| (2,694) | 1:77:A:ASN:HD22 | 1:64:A:ARG:H | 6 | 0.16 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 4 | 0.16 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 6 | 0.16 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 16 | 0.16 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 18 | 0.16 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 20 | 0.16 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 13 | 0.16 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 9 | 0.16 |
| (2,594) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 2 | 0.16 |
| (2,550) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 7 | 0.16 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 10 | 0.16 |
| (2,487) | 1:57:A:VAL:HG21 | 1:58:A:GLU:H | 7 | 0.16 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 6 | 0.16 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 9 | 0.16 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 11 | 0.16 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 15 | 0.16 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 19 | 0.16 |
| (2,453) | 1:34:A:VAL:HB | 1:35:A:LYS:H | 17 | 0.16 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 12 | 0.16 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 15 | 0.16 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 5 | 0.16 |
| (2,268) | 1:14:A:VAL:HG23 | 1:21:A:LEU:H | 18 | 0.16 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 6 | 0.16 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 12 | 0.16 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG23 | 16 | 0.16 |
| (2,236) | 1:21:A:LEU:H | 1:22:A:ILE:HG21 | 17 | 0.16 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 4 | 0.16 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 8 | 0.16 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 19 | 0.16 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 8 | 0.16 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 13 | 0.16 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 14 | 0.16 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 11 | 0.16 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 18 | 0.16 |
| (2,96) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 1 | 0.16 |
| (2,91) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 11 | 0.16 |
| (2,85) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 1 | 0.16 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 17 | 0.16 |
| (2,41) | 1:96:A:VAL:HG11 | 1:148:A:ALA:H | 9 | 0.16 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 16 | 0.16 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 14 | 0.16 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 18 | 0.16 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 2 | 0.16 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 5 | 0.16 |
| (1,118) | 1:168:A:ILE:N | 1:122:A:VAL:O | 9 | 0.16 |
| (1,117) | 1:168:A:ILE:H | 1:122:A:VAL:O | 15 | 0.16 |
| (1,111) | 1:159:A:TYR:H | 1:167:A:LEU:O | 18 | 0.16 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 15 | 0.16 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 3 | 0.16 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 11 | 0.16 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 5 | 0.16 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 19 | 0.16 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 11 | 0.16 |
| (1,89) | 1:132:A:ARG:H | 1:128:A:ILE:O | 12 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 13 | 0.16 |
| (1,77) | 1:112:A:ASP:H | 1:108:A:LEU:O | 1 | 0.16 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 2 | 0.16 |
| (1,59) | 1:77:A:ASN:H | 1:64:A:ARG:O | 3 | 0.16 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 7 | 0.16 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 9 | 0.16 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 12 | 0.16 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 6 | 0.16 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 10 | 0.16 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 8 | 0.16 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 3 | 0.16 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 8 | 0.16 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 11 | 0.16 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 12 | 0.16 |
| (1,34) | 1:42:A:LYS:N | 1:38:A:LEU:O | 5 | 0.16 |
| (1,30) | 1:40:A:LYS:N | 1:36:A:GLU:O | 13 | 0.16 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 10 | 0.16 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 3 | 0.16 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 19 | 0.16 |
| (1,24) | 1:37:A:LEU:N | 1:33:A:PRO:O | 2 | 0.16 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 6 | 0.16 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 3 | 0.16 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 11 | 0.16 |
| (1,10) | 1:11:A:LEU:N | 1:7:A:VAL:O | 18 | 0.16 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 1 | 0.16 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 5 | 0.16 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 16 | 0.16 |
| (1,6) | 1:9:A:LYS:N | 1:5:A:VAL:O | 2 | 0.16 |
| (1,4) | 1:8:A:SER:N | 1:4:A:MET:O | 11 | 0.16 |
| (1,2) | 1:7:A:VAL:N | 1:3:A:HIS:O | 12 | 0.16 |
| (4,458) | 1:50:A:MET:HE1 | 1:51:A:GLU:HA | 2 | 0.15 |
| (4,452) | 1:92:A:VAL:HA | 1:92:A:VAL:HG12 | 14 | 0.15 |
| (4,448) | 1:110:A:LEU:HD21 | 1:144:A:LEU:HG | 9 | 0.15 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 5 | 0.15 |
| (4,311) | 1:143:A:VAL:HG12 | 1:178:A:VAL:HA | 17 | 0.15 |
| (4,307) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 13 | 0.15 |
| (4,299) | 1:168:A:ILE:HD12 | 1:152:A:ALA:HA | 4 | 0.15 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 9 | 0.15 |
| (4,259) | 1:117:A:MET:HE1 | 2:201:A:NAD:H2A | 16 | 0.15 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 18 | 0.15 |
| (4,223) | 1:13:A:LEU:HD12 | 1:10:A:PHE:HE1 | 12 | 0.15 |
| (4,195) | 1:114:A:ILE:HD11 | 1:117:A:MET:HE1 | 12 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 9 | 0.15 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 14 | 0.15 |
| (4,61) | 1:37:A:LEU:H | 1:38:A:LEU:HD23 | 4 | 0.15 |
| (4,61) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 9 | 0.15 |
| (4,37) | 1:66:A:ALA:H | 1:57:A:VAL:HG13 | 12 | 0.15 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 16 | 0.15 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 19 | 0.15 |
| (4,7) | 1:13:A:LEU:HD11 | 1:10:A:PHE:HE1 | 17 | 0.15 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD22 | 20 | 0.15 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 2 | 0.15 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 7 | 0.15 |
| (2,3920) | 1:115:A:LYS:H | 2:201:A:NAD:H8A | 3 | 0.15 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 10 | 0.15 |
| (2,3884) | 2:201:A:NAD:H1B | 1:109:A:ILE:HD12 | 17 | 0.15 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 1 | 0.15 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 3 | 0.15 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 4 | 0.15 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 12 | 0.15 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 1 | 0.15 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 10 | 0.15 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 11 | 0.15 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 17 | 0.15 |
| (2,3837) | 1:5:A:VAL:HG22 | 1:5:A:VAL:HA | 14 | 0.15 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 4 | 0.15 |
| (2,3835) | 1:168:A:ILE:HG23 | 1:168:A:ILE:HD11 | 13 | 0.15 |
| (2,3832) | 1:97:A:LEU:HD23 | 1:151:A:MET:HG3 | 1 | 0.15 |
| (2,3825) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB2 | 17 | 0.15 |
| (2,3819) | 1:151:A:MET:HE1 | 1:171:A:VAL:HG12 | 17 | 0.15 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 1 | 0.15 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 11 | 0.15 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 16 | 0.15 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 9 | 0.15 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 13 | 0.15 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 1 | 0.15 |
| (2,3793) | 1:53:A:LEU:HD21 | 1:56:A:ILE:HB | 2 | 0.15 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 3 | 0.15 |
| (2,3793) | 1:53:A:LEU:HD23 | 1:56:A:ILE:HB | 15 | 0.15 |
| (2,3785) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HG2 | 8 | 0.15 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 17 | 0.15 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 2 | 0.15 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 3 | 0.15 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 4 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 6 | 0.15 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 7 | 0.15 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 15 | 0.15 |
| (2,3770) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 2 | 0.15 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 5 | 0.15 |
| (2,3770) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 7 | 0.15 |
| (2,3770) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 9 | 0.15 |
| (2,3770) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 11 | 0.15 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 19 | 0.15 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 7 | 0.15 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 8 | 0.15 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 10 | 0.15 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 14 | 0.15 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 7 | 0.15 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 2 | 0.15 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 16 | 0.15 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 18 | 0.15 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 20 | 0.15 |
| (2,3679) | 1:97:A:LEU:HD23 | 1:97:A:LEU:HA | 2 | 0.15 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 9 | 0.15 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 10 | 0.15 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 12 | 0.15 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 13 | 0.15 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 16 | 0.15 |
| (2,3575) | 1:50:A:MET:HE2 | 1:50:A:MET:HG3 | 2 | 0.15 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 3 | 0.15 |
| (2,3518) | 1:128:A:ILE:HD13 | 1:128:A:ILE:HA | 14 | 0.15 |
| (2,3500) | 1:144:A:LEU:HD23 | 1:145:A:SER:HB2 | 20 | 0.15 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 3 | 0.15 |
| (2,3495) | 1:82:A:VAL:HG22 | 1:82:A:VAL:HA | 8 | 0.15 |
| (2,3493) | 1:142:A:VAL:HG23 | 1:178:A:VAL:HA | 1 | 0.15 |
| (2,3479) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 2 | 0.15 |
| (2,3478) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 12 | 0.15 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 10 | 0.15 |
| (2,3445) | 1:97:A:LEU:HD21 | 1:166:A:TRP:HE3 | 6 | 0.15 |
| (2,3409) | 1:84:A:VAL:HG13 | 1:85:A:ASP:H | 3 | 0.15 |
| (2,3405) | 1:56:A:ILE:HG21 | 1:57:A:VAL:H | 14 | 0.15 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 4 | 0.15 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 7 | 0.15 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 13 | 0.15 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 4 | 0.15 |
| (2,3288) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 14 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 3 | 0.15 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 15 | 0.15 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 5 | 0.15 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 7 | 0.15 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 9 | 0.15 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 16 | 0.15 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 7 | 0.15 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 13 | 0.15 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 14 | 0.15 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 19 | 0.15 |
| (2,3159) | 1:176:A:ILE:HG21 | 1:178:A:VAL:H | 14 | 0.15 |
| (2,3127) | 1:97:A:LEU:HD13 | 1:124:A:LEU:HD21 | 11 | 0.15 |
| (2,2853) | 1:86:A:LEU:HD11 | 1:86:A:LEU:H | 20 | 0.15 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 4 | 0.15 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 11 | 0.15 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 1 | 0.15 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 4 | 0.15 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 11 | 0.15 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 5 | 0.15 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 5 | 0.15 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 9 | 0.15 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 5 | 0.15 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 1 | 0.15 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 13 | 0.15 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 9 | 0.15 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 16 | 0.15 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 20 | 0.15 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 2 | 0.15 |
| (2,2367) | 1:48:A:ILE:HG23 | 1:48:A:ILE:H | 6 | 0.15 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 19 | 0.15 |
| (2,2296) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 17 | 0.15 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 9 | 0.15 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 14 | 0.15 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 6 | 0.15 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 8 | 0.15 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 10 | 0.15 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 13 | 0.15 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 14 | 0.15 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 17 | 0.15 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 18 | 0.15 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 19 | 0.15 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 16 | 0.15 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 20 | 0.15 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 18 | 0.15 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 8 | 0.15 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 18 | 0.15 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 5 | 0.15 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 9 | 0.15 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 12 | 0.15 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 16 | 0.15 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 1 | 0.15 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 5 | 0.15 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 17 | 0.15 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 20 | 0.15 |
| (2,1973) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 7 | 0.15 |
| (2,1973) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 11 | 0.15 |
| (2,1973) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 18 | 0.15 |
| (2,1973) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 20 | 0.15 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 8 | 0.15 |
| (2,1962) | 1:110:A:LEU:HD13 | 1:106:A:PHE:HE1 | 9 | 0.15 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 17 | 0.15 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 20 | 0.15 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 1 | 0.15 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 8 | 0.15 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 9 | 0.15 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 12 | 0.15 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 15 | 0.15 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 16 | 0.15 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 16 | 0.15 |
| (2,1809) | 1:34:A:VAL:HG13 | 1:37:A:LEU:HB3 | 1 | 0.15 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 14 | 0.15 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 14 | 0.15 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 17 | 0.15 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 1 | 0.15 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 4 | 0.15 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 12 | 0.15 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 11 | 0.15 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 17 | 0.15 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 19 | 0.15 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 20 | 0.15 |
| (2,1745) | 1:34:A:VAL:HA | 1:37:A:LEU:HD21 | 17 | 0.15 |
| (2,1741) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 1 | 0.15 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 17 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1633) | 1:42:A:LYS:HE2 | 1:39:A:ALA:HA | 13 | 0.15 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 9 | 0.15 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 10 | 0.15 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 13 | 0.15 |
| (2,1599) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 3 | 0.15 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 3 | 0.15 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 16 | 0.15 |
| (2,1455) | 1:165:A:VAL:HG23 | 2:201:A:NAD:H5N | 15 | 0.15 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 8 | 0.15 |
| (2,1410) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 12 | 0.15 |
| (2,1410) | 1:95:A:ALA:HB3 | 1:96:A:VAL:H | 19 | 0.15 |
| (2,1399) | 1:86:A:LEU:HG | 1:86:A:LEU:H | 1 | 0.15 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 13 | 0.15 |
| (2,1301) | 1:34:A:VAL:HG11 | 1:38:A:LEU:H | 5 | 0.15 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 11 | 0.15 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 2 | 0.15 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 3 | 0.15 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 4 | 0.15 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 13 | 0.15 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 19 | 0.15 |
| (2,1274) | 1:160:A:LEU:HD22 | 1:91:A:GLN:HE22 | 6 | 0.15 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 2 | 0.15 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 10 | 0.15 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 16 | 0.15 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 19 | 0.15 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 4 | 0.15 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 9 | 0.15 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 19 | 0.15 |
| (2,1218) | 1:177:A:LYS:HG2 | 1:177:A:LYS:HA | 7 | 0.15 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 1 | 0.15 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 4 | 0.15 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 15 | 0.15 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 16 | 0.15 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 17 | 0.15 |
| (2,1194) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 18 | 0.15 |
| (2,1075) | 1:56:A:ILE:H | 1:58:A:GLU:H | 17 | 0.15 |
| (2,1066) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 12 | 0.15 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 2 | 0.15 |
| (2,1021) | 1:37:A:LEU:H | 1:34:A:VAL:H | 4 | 0.15 |
| (2,1014) | 1:160:A:LEU:H | 1:89:A:GLU:H | 3 | 0.15 |
| (2,1012) | 1:40:A:LYS:H | 1:39:A:ALA:H | 15 | 0.15 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 4 | 0.15 |
| (2,969) | 1:23:A:GLY:H | 1:22:A:ILE:H | 20 | 0.15 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 17 | 0.15 |
| (2,908) | 1:96:A:VAL:H | 1:97:A:LEU:H | 14 | 0.15 |
| (2,810) | 1:22:A:ILE:H | 1:37:A:LEU:HD12 | 19 | 0.15 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 13 | 0.15 |
| (2,708) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 20 | 0.15 |
| (2,681) | 1:78:A:GLN:HE21 | 1:76:A:ALA:HA | 1 | 0.15 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 2 | 0.15 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 6 | 0.15 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 3 | 0.15 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 10 | 0.15 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 13 | 0.15 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 14 | 0.15 |
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB3 | 17 | 0.15 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 9 | 0.15 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 10 | 0.15 |
| (2,546) | 1:114:A:ILE:HD11 | 1:114:A:ILE:H | 17 | 0.15 |
| (2,453) | 1:34:A:VAL:HB | 1:35:A:LYS:H | 15 | 0.15 |
| (2,445) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 13 | 0.15 |
| (2,431) | 1:73:A:LYS:H | 1:34:A:VAL:HG21 | 14 | 0.15 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 12 | 0.15 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 14 | 0.15 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 6 | 0.15 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 8 | 0.15 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 12 | 0.15 |
| (2,268) | 1:14:A:VAL:HG23 | 1:21:A:LEU:H | 6 | 0.15 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 7 | 0.15 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 14 | 0.15 |
| (2,198) | 1:20:A:ALA:HA | 1:24:A:LEU:H | 20 | 0.15 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 12 | 0.15 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 1 | 0.15 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 6 | 0.15 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 18 | 0.15 |
| (2,138) | 1:83:A:GLU:H | 1:85:A:ASP:H | 19 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 3 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 4 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 5 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 6 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 7 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 9 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 12 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 15 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 16 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 17 | 0.15 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 19 | 0.15 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 9 | 0.15 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 5 | 0.15 |
| (2,85) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 8 | 0.15 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 16 | 0.15 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 18 | 0.15 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 9 | 0.15 |
| (1,119) | 1:171:A:VAL:H | 1:114:A:ILE:O | 20 | 0.15 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 10 | 0.15 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 15 | 0.15 |
| (1,110) | 1:153:A:ASP:N | 1:149:A:LYS:O | 13 | 0.15 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 18 | 0.15 |
| (1,102) | 1:144:A:LEU:N | 1:99:A:HIS:O | 2 | 0.15 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 9 | 0.15 |
| (1,77) | 1:112:A:ASP:H | 1:108:A:LEU:O | 10 | 0.15 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 18 | 0.15 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 19 | 0.15 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 7 | 0.15 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 12 | 0.15 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 16 | 0.15 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 18 | 0.15 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 3 | 0.15 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 14 | 0.15 |
| (1,55) | 1:74:A:ILE:H | 1:32:A:ALA:O | 18 | 0.15 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 5 | 0.15 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 15 | 0.15 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 7 | 0.15 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 10 | 0.15 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 2 | 0.15 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 6 | 0.15 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 15 | 0.15 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 18 | 0.15 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 6 | 0.15 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 9 | 0.15 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 17 | 0.15 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 19 | 0.15 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 1 | 0.15 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 20 | 0.15 |
| (1,22) | 1:32:A:ALA:N | 1:74:A:ILE:O | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 4 | 0.15 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 16 | 0.15 |
| (1,17) | 1:15:A:LEU:H | 1:11:A:LEU:O | 20 | 0.15 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 19 | 0.15 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 10 | 0.15 |
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 15 | 0.15 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 9 | 0.15 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 13 | 0.15 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 18 | 0.14 |
| (4,425) | 1:34:A:VAL:HG21 | 1:35:A:LYS:HB2 | 12 | 0.14 |
| (4,392) | 1:8:A:SER:HB2 | 1:7:A:VAL:HB | 1 | 0.14 |
| (4,388) | 1:107:A:ASP:HA | 1:110:A:LEU:HD23 | 12 | 0.14 |
| (4,307) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 4 | 0.14 |
| (4,300) | 1:97:A:LEU:HD23 | 1:156:A:PHE:HB3 | 20 | 0.14 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 11 | 0.14 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HZ | 8 | 0.14 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 9 | 0.14 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 19 | 0.14 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 17 | 0.14 |
| (4,61) | 1:37:A:LEU:H | 1:24:A:LEU:HD12 | 6 | 0.14 |
| (4,59) | 1:40:A:LYS:H | 1:44:A:LYS:HE2 | 7 | 0.14 |
| (4,41) | 1:5:A:VAL:HG21 | 1:5:A:VAL:H | 9 | 0.14 |
| (4,41) | 1:5:A:VAL:HG23 | 1:5:A:VAL:H | 12 | 0.14 |
| (4,25) | 1:75:A:ARG:H | 1:74:A:ILE:HG12 | 8 | 0.14 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 4 | 0.14 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 11 | 0.14 |
| (2,3940) | 1:134:A:VAL:HG11 | 2:201:A:NAD:H2N | 19 | 0.14 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 16 | 0.14 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 20 | 0.14 |
| (2,3918) | 1:114:A:ILE:HD11 | 2:201:A:NAD:H8A | 6 | 0.14 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 6 | 0.14 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 15 | 0.14 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 2 | 0.14 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 4 | 0.14 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 7 | 0.14 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 12 | 0.14 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 20 | 0.14 |
| (2,3837) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 1 | 0.14 |
| (2,3828) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 19 | 0.14 |
| (2,3819) | 1:151:A:MET:HE3 | 1:171:A:VAL:HG12 | 12 | 0.14 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD13 | 6 | 0.14 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3812) | 1:56:A:ILE:HG21 | 1:11:A:LEU:HD11 | 9 | 0.14 |
| (2,3811) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 1 | 0.14 |
| (2,3809) | 1:110:A:LEU:HD12 | 1:176:A:ILE:HB | 18 | 0.14 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 10 | 0.14 |
| (2,3802) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 18 | 0.14 |
| (2,3802) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 20 | 0.14 |
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 16 | 0.14 |
| (2,3794) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HB | 13 | 0.14 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 19 | 0.14 |
| (2,3770) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 8 | 0.14 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 10 | 0.14 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 3 | 0.14 |
| (2,3763) | 1:76:A:ALA:HB1 | 1:15:A:LEU:HD11 | 7 | 0.14 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 11 | 0.14 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 13 | 0.14 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 18 | 0.14 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 19 | 0.14 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 5 | 0.14 |
| (2,3707) | 1:11:A:LEU:HA | 1:37:A:LEU:HD21 | 5 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 1 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 4 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 5 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 8 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 9 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 11 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 12 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 13 | 0.14 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 14 | 0.14 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 5 | 0.14 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 18 | 0.14 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 19 | 0.14 |
| (2,3575) | 1:50:A:MET:HE1 | 1:50:A:MET:HG3 | 4 | 0.14 |
| (2,3575) | 1:50:A:MET:HE3 | 1:50:A:MET:HG3 | 18 | 0.14 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 8 | 0.14 |
| (2,3519) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 16 | 0.14 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 19 | 0.14 |
| (2,3518) | 1:128:A:ILE:HD12 | 1:128:A:ILE:HA | 7 | 0.14 |
| (2,3518) | 1:128:A:ILE:HD11 | 1:128:A:ILE:HA | 15 | 0.14 |
| (2,3510) | 1:144:A:LEU:HD23 | 1:106:A:PHE:HB2 | 12 | 0.14 |
| (2,3509) | 1:13:A:LEU:HD21 | 1:17:A:HIS:HB2 | 4 | 0.14 |
| (2,3483) | 1:26:A:LEU:HD13 | 1:32:A:ALA:HA | 13 | 0.14 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 19 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3434) | 1:15:A:LEU:HD12 | 1:65:A:PHE:HE1 | 2 | 0.14 |
| (2,3434) | 1:15:A:LEU:HD12 | 1:65:A:PHE:HE1 | 14 | 0.14 |
| (2,3424) | 1:165:A:VAL:HG23 | 2:201:A:NAD:H5N | 19 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 5 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 7 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 8 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG23 | 1:57:A:VAL:H | 9 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 12 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 16 | 0.14 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 20 | 0.14 |
| (2,3390) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 5 | 0.14 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 5 | 0.14 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 17 | 0.14 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 18 | 0.14 |
| (2,3370) | 1:152:A:ALA:HB3 | 1:158:A:PHE:HD1 | 14 | 0.14 |
| (2,3362) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 20 | 0.14 |
| (2,3355) | 1:41:A:MET:HE2 | 1:41:A:MET:H | 16 | 0.14 |
| (2,3345) | 1:41:A:MET:HE1 | 1:10:A:PHE:HE1 | 9 | 0.14 |
| (2,3288) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 15 | 0.14 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 16 | 0.14 |
| (2,3248) | 1:160:A:LEU:HD22 | 1:91:A:GLN:HE22 | 6 | 0.14 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 13 | 0.14 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD21 | 14 | 0.14 |
| (2,3102) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 2 | 0.14 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 1 | 0.14 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 9 | 0.14 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 15 | 0.14 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 16 | 0.14 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 18 | 0.14 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 19 | 0.14 |
| (2,2949) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 8 | 0.14 |
| (2,2887) | 1:176:A:ILE:H | 1:146:A:VAL:HG11 | 9 | 0.14 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 9 | 0.14 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 13 | 0.14 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 6 | 0.14 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 18 | 0.14 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 3 | 0.14 |
| (2,2651) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE22 | 1 | 0.14 |
| (2,2651) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE22 | 11 | 0.14 |
| (2,2649) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 15 | 0.14 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 1 | 0.14 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 9 | 0.14 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 12 | 0.14 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 14 | 0.14 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 1 | 0.14 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 4 | 0.14 |
| (2,2566) | 1:43:A:ALA:HB3 | 1:44:A:LYS:H | 15 | 0.14 |
| (2,2521) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 6 | 0.14 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 13 | 0.14 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 5 | 0.14 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 2 | 0.14 |
| (2,2234) | 1:14:A:VAL:HG23 | 1:21:A:LEU:H | 18 | 0.14 |
| (2,2216) | 1:26:A:LEU:HD11 | 1:27:A:ASP:H | 20 | 0.14 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 13 | 0.14 |
| (2,2175) | 1:57:A:VAL:HG21 | 1:66:A:ALA:H | 8 | 0.14 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD22 | 4 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 4 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 5 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 7 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 9 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 12 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 15 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 16 | 0.14 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 20 | 0.14 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 7 | 0.14 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 2 | 0.14 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 3 | 0.14 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 5 | 0.14 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 9 | 0.14 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 17 | 0.14 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 10 | 0.14 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 3 | 0.14 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 12 | 0.14 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 19 | 0.14 |
| (2,2106) | 1:84:A:VAL:HB | 1:85:A:ASP:H | 5 | 0.14 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 2 | 0.14 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 2 | 0.14 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 15 | 0.14 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 2 | 0.14 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 15 | 0.14 |
| (2,1973) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 8 | 0.14 |
| (2,1973) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 9 | 0.14 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 11 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 19 | 0.14 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 2 | 0.14 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 15 | 0.14 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 16 | 0.14 |
| (2,1860) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 4 | 0.14 |
| (2,1860) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 18 | 0.14 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 4 | 0.14 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 6 | 0.14 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD12 | 9 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 2 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 9 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 10 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 14 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 15 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 16 | 0.14 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 17 | 0.14 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 2 | 0.14 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 14 | 0.14 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 2 | 0.14 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 3 | 0.14 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 6 | 0.14 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 15 | 0.14 |
| (2,1805) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 4 | 0.14 |
| (2,1805) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 6 | 0.14 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 15 | 0.14 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 18 | 0.14 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 5 | 0.14 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 10 | 0.14 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 20 | 0.14 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD22 | 5 | 0.14 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 11 | 0.14 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 17 | 0.14 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 5 | 0.14 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 6 | 0.14 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 7 | 0.14 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 11 | 0.14 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 12 | 0.14 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG23 | 17 | 0.14 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 3 | 0.14 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 5 | 0.14 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 6 | 0.14 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 14 | 0.14 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 17 | 0.14 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 20 | 0.14 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 9 | 0.14 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 10 | 0.14 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 13 | 0.14 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 14 | 0.14 |
| (2,1723) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 5 | 0.14 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 5 | 0.14 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 10 | 0.14 |
| (2,1710) | 1:26:A:LEU:HD23 | 1:15:A:LEU:HA | 7 | 0.14 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 17 | 0.14 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 5 | 0.14 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 12 | 0.14 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 13 | 0.14 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 16 | 0.14 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 19 | 0.14 |
| (2,1599) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 6 | 0.14 |
| (2,1599) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 13 | 0.14 |
| (2,1590) | 1:32:A:ALA:HB2 | 1:33:A:PRO:HD3 | 18 | 0.14 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 4 | 0.14 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 11 | 0.14 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 20 | 0.14 |
| (2,1514) | 1:124:A:LEU:HD11 | 1:167:A:LEU:HA | 4 | 0.14 |
| (2,1509) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 1 | 0.14 |
| (2,1474) | 1:110:A:LEU:HD23 | 1:110:A:LEU:H | 6 | 0.14 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 7 | 0.14 |
| (2,1474) | 1:110:A:LEU:HD21 | 1:110:A:LEU:H | 13 | 0.14 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 9 | 0.14 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 4 | 0.14 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 10 | 0.14 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 15 | 0.14 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 17 | 0.14 |
| (2,1425) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HD1 | 20 | 0.14 |
| (2,1420) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HE1 | 2 | 0.14 |
| (2,1399) | 1:86:A:LEU:HG | 1:86:A:LEU:H | 6 | 0.14 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 11 | 0.14 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 18 | 0.14 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 5 | 0.14 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 18 | 0.14 |
| (2,1283) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 4 | 0.14 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 3 | 0.14 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 8 | 0.14 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 15 | 0.14 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 8 | 0.14 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 10 | 0.14 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 11 | 0.14 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 14 | 0.14 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 15 | 0.14 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 16 | 0.14 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 17 | 0.14 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 11 | 0.14 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 5 | 0.14 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 12 | 0.14 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 14 | 0.14 |
| (2,1158) | 1:165:A:VAL:HG21 | 1:165:A:VAL:H | 18 | 0.14 |
| (2,1158) | 1:165:A:VAL:HG21 | 1:165:A:VAL:H | 19 | 0.14 |
| (2,1104) | 1:18:A:ASN:H | 1:27:A:ASP:H | 17 | 0.14 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 11 | 0.14 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 17 | 0.14 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 3 | 0.14 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 13 | 0.14 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 15 | 0.14 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 20 | 0.14 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 7 | 0.14 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 13 | 0.14 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 7 | 0.14 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 11 | 0.14 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 14 | 0.14 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 18 | 0.14 |
| (2,723) | 1:20:A:ALA:HA | 1:23:A:GLY:H | 1 | 0.14 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 7 | 0.14 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 17 | 0.14 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 1 | 0.14 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 2 | 0.14 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 3 | 0.14 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 15 | 0.14 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 16 | 0.14 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG11 | 1 | 0.14 |
| (2,431) | 1:73:A:LYS:H | 1:34:A:VAL:HG21 | 7 | 0.14 |
| (2,431) | 1:73:A:LYS:H | 1:34:A:VAL:HG21 | 15 | 0.14 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 19 | 0.14 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 5 | 0.14 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 16 | 0.14 |
| (2,297) | 1:50:A:MET:H | 1:50:A:MET:HB3 | 4 | 0.14 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 8 | 0.14 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 17 | 0.14 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 13 | 0.14 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 17 | 0.14 |
| (2,205) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 15 | 0.14 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 7 | 0.14 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 11 | 0.14 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 19 | 0.14 |
| (2,187) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 6 | 0.14 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 16 | 0.14 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 5 | 0.14 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 4 | 0.14 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 12 | 0.14 |
| (2,134) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 7 | 0.14 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 1 | 0.14 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 2 | 0.14 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 8 | 0.14 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 10 | 0.14 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 13 | 0.14 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 14 | 0.14 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 18 | 0.14 |
| (2,129) | 1:173:A:ALA:HA | 1:173:A:ALA:H | 20 | 0.14 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 6 | 0.14 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 12 | 0.14 |
| (2,62) | 1:178:A:VAL:H | 1:177:A:LYS:H | 11 | 0.14 |
| (2,19) | 1:13:A:LEU:HA | 1:17:A:HIS:HD2 | 12 | 0.14 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 8 | 0.14 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 7 | 0.14 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 10 | 0.14 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 13 | 0.14 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 18 | 0.14 |
| (1,118) | 1:168:A:ILE:N | 1:122:A:VAL:O | 18 | 0.14 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 20 | 0.14 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 2 | 0.14 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 14 | 0.14 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 6 | 0.14 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 4 | 0.14 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 9 | 0.14 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 14 | 0.14 |
| (1,55) | 1:74:A:ILE:H | 1:32:A:ALA:O | 17 | 0.14 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 9 | 0.14 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 16 | 0.14 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 19 | 0.14 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 19 | 0.14 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 2 | 0.14 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 4 | 0.14 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 15 | 0.14 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 19 | 0.14 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 11 | 0.14 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 13 | 0.14 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 17 | 0.14 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 20 | 0.14 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 6 | 0.14 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 10 | 0.14 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 18 | 0.14 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 13 | 0.14 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 14 | 0.14 |
| (1,4) | 1:8:A:SER:N | 1:4:A:MET:O | 14 | 0.14 |
| (1,4) | 1:8:A:SER:N | 1:4:A:MET:O | 17 | 0.14 |
| (1,1) | 1:7:A:VAL:H | 1:3:A:HIS:O | 7 | 0.14 |
| (4,459) | 1:94:A:PRO:HA | 1:151:A:MET:HB2 | 6 | 0.13 |
| (4,443) | 1:48:A:ILE:HD12 | 1:38:A:LEU:HB2 | 17 | 0.13 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 14 | 0.13 |
| (4,442) | 1:178:A:VAL:HG21 | 1:144:A:LEU:HG | 19 | 0.13 |
| (4,436) | 1:34:A:VAL:HG12 | 1:35:A:LYS:HG3 | 15 | 0.13 |
| (4,379) | 1:50:A:MET:HA | 1:39:A:ALA:HB3 | 1 | 0.13 |
| (4,353) | 1:143:A:VAL:HB | 1:131:A:ALA:HA | 2 | 0.13 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 8 | 0.13 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HE1 | 6 | 0.13 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HZ | 9 | 0.13 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HZ | 15 | 0.13 |
| (4,259) | 1:117:A:MET:HE3 | 2:201:A:NAD:H2A | 18 | 0.13 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 6 | 0.13 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 8 | 0.13 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 12 | 0.13 |
| (4,213) | 1:165:A:VAL:HB | 1:123:A:HIS:HA | 16 | 0.13 |
| (4,198) | 1:176:A:ILE:HD13 | 1:106:A:PHE:HE1 | 11 | 0.13 |
| (4,173) | 1:52:A:GLU:H | 1:58:A:GLU:H | 13 | 0.13 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 18 | 0.13 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,65) | 1:7:A:VAL:H | 1:7:A:VAL:HB | 1 | 0.13 |
| (4,65) | 1:7:A:VAL:H | 1:7:A:VAL:HB | 8 | 0.13 |
| (4,41) | 1:5:A:VAL:HG22 | 1:5:A:VAL:H | 1 | 0.13 |
| (4,41) | 1:5:A:VAL:HG22 | 1:5:A:VAL:H | 8 | 0.13 |
| (4,41) | 1:5:A:VAL:HG22 | 1:5:A:VAL:H | 16 | 0.13 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD22 | 9 | 0.13 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 12 | 0.13 |
| (3,20) | 1:163:A:ASN:OD1 | 2:201:A:NAD:H71N | 2 | 0.13 |
| (2,3947) | 1:165:A:VAL:HG21 | 2:201:A:NAD:H4N | 18 | 0.13 |
| (2,3937) | 1:105:A:ASN:HD21 | 2:201:A:NAD:HO2A | 20 | 0.13 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 15 | 0.13 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 17 | 0.13 |
| (2,3918) | 1:114:A:ILE:HD11 | 2:201:A:NAD:H8A | 19 | 0.13 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 8 | 0.13 |
| (2,3896) | 2:201:A:NAD:H3D | 2:201:A:NAD:H2N | 10 | 0.13 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 17 | 0.13 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 3 | 0.13 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 3 | 0.13 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 13 | 0.13 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 15 | 0.13 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 19 | 0.13 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 7 | 0.13 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 15 | 0.13 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 16 | 0.13 |
| (2,3837) | 1:5:A:VAL:HG21 | 1:5:A:VAL:HA | 12 | 0.13 |
| (2,3826) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 20 | 0.13 |
| (2,3825) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB2 | 10 | 0.13 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 2 | 0.13 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 3 | 0.13 |
| (2,3802) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 2 | 0.13 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 12 | 0.13 |
| (2,3802) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 14 | 0.13 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 4 | 0.13 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 10 | 0.13 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 10 | 0.13 |
| (2,3773) | 1:34:A:VAL:HG13 | 1:37:A:LEU:HB3 | 18 | 0.13 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 14 | 0.13 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 16 | 0.13 |
| (2,3770) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 17 | 0.13 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 6 | 0.13 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 15 | 0.13 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 11 | 0.13 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 15 | 0.13 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 16 | 0.13 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 8 | 0.13 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 14 | 0.13 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 17 | 0.13 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 20 | 0.13 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 7 | 0.13 |
| (2,3575) | 1:50:A:MET:HE1 | 1:50:A:MET:HG3 | 6 | 0.13 |
| (2,3575) | 1:50:A:MET:HE1 | 1:50:A:MET:HG3 | 10 | 0.13 |
| (2,3570) | 1:4:A:MET:HE1 | 1:52:A:GLU:HA | 9 | 0.13 |
| (2,3478) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 5 | 0.13 |
| (2,3474) | 1:146:A:VAL:HG13 | 1:96:A:VAL:HA | 16 | 0.13 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 1 | 0.13 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 6 | 0.13 |
| (2,3468) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HA | 1 | 0.13 |
| (2,3459) | 1:167:A:LEU:HD23 | 1:123:A:HIS:HA | 9 | 0.13 |
| (2,3409) | 1:84:A:VAL:HG11 | 1:85:A:ASP:H | 14 | 0.13 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 13 | 0.13 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 17 | 0.13 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 19 | 0.13 |
| (2,3390) | 1:56:A:ILE:HG21 | 1:65:A:PHE:HE1 | 14 | 0.13 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 1 | 0.13 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 6 | 0.13 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 11 | 0.13 |
| (2,3362) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 15 | 0.13 |
| (2,3335) | 1:16:A:ARG:HD2 | 1:12:A:SER:H | 4 | 0.13 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 3 | 0.13 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 5 | 0.13 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 12 | 0.13 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 15 | 0.13 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 2 | 0.13 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 9 | 0.13 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 6 | 0.13 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 15 | 0.13 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 17 | 0.13 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 19 | 0.13 |
| (2,3211) | 1:151:A:MET:HE3 | 1:156:A:PHE:HZ | 5 | 0.13 |
| (2,3180) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 8 | 0.13 |
| (2,3102) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 3 | 0.13 |
| (2,3036) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 14 | 0.13 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 6 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 10 | 0.13 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 11 | 0.13 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 14 | 0.13 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 7 | 0.13 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 4 | 0.13 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 9 | 0.13 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 11 | 0.13 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 16 | 0.13 |
| (2,2722) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 13 | 0.13 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 8 | 0.13 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 18 | 0.13 |
| (2,2651) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE22 | 3 | 0.13 |
| (2,2651) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE22 | 10 | 0.13 |
| (2,2651) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE22 | 12 | 0.13 |
| (2,2651) | 1:78:A:GLN:HG3 | 1:78:A:GLN:HE22 | 14 | 0.13 |
| (2,2649) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 11 | 0.13 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 5 | 0.13 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 20 | 0.13 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 16 | 0.13 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 17 | 0.13 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 5 | 0.13 |
| (2,2566) | 1:43:A:ALA:HB1 | 1:44:A:LYS:H | 12 | 0.13 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 18 | 0.13 |
| (2,2566) | 1:43:A:ALA:HB3 | 1:44:A:LYS:H | 19 | 0.13 |
| (2,2550) | 1:86:A:LEU:H | 1:88:A:TYR:H | 7 | 0.13 |
| (2,2506) | 1:64:A:ARG:H | 1:76:A:ALA:HB1 | 4 | 0.13 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 6 | 0.13 |
| (2,2367) | 1:48:A:ILE:HG21 | 1:48:A:ILE:H | 14 | 0.13 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 5 | 0.13 |
| (2,2268) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 2 | 0.13 |
| (2,2232) | 1:21:A:LEU:H | 1:24:A:LEU:HD21 | 12 | 0.13 |
| (2,2210) | 1:48:A:ILE:HD12 | 1:53:A:LEU:H | 14 | 0.13 |
| (2,2210) | 1:48:A:ILE:HD11 | 1:53:A:LEU:H | 18 | 0.13 |
| (2,2210) | 1:48:A:ILE:HD12 | 1:53:A:LEU:H | 19 | 0.13 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 5 | 0.13 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 7 | 0.13 |
| (2,2175) | 1:57:A:VAL:HG21 | 1:66:A:ALA:H | 19 | 0.13 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 1 | 0.13 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 2 | 0.13 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 11 | 0.13 |
| (2,2151) | 1:13:A:LEU:H | 1:13:A:LEU:HB3 | 12 | 0.13 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 12 | 0.13 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 13 | 0.13 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 17 | 0.13 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 19 | 0.13 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 9 | 0.13 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 1 | 0.13 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 8 | 0.13 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 10 | 0.13 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 19 | 0.13 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 3 | 0.13 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 12 | 0.13 |
| (2,2010) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 6 | 0.13 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 12 | 0.13 |
| (2,1962) | 1:110:A:LEU:HD11 | 1:106:A:PHE:HE1 | 16 | 0.13 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 6 | 0.13 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 9 | 0.13 |
| (2,1934) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 16 | 0.13 |
| (2,1932) | 2:201:A:NAD:H3D | 2:201:A:NAD:H2N | 10 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 1 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 2 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 3 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 5 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 9 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 10 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 12 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 15 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 16 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 18 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 19 | 0.13 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 20 | 0.13 |
| (2,1880) | 1:76:A:ALA:HB1 | 1:16:A:ARG:HA | 5 | 0.13 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 7 | 0.13 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 13 | 0.13 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 18 | 0.13 |
| (2,1867) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 12 | 0.13 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 3 | 0.13 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 10 | 0.13 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 15 | 0.13 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 2 | 0.13 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 5 | 0.13 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG22 | 13 | 0.13 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 16 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG21 | 19 | 0.13 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 19 | 0.13 |
| (2,1842) | 1:11:A:LEU:HD22 | 1:11:A:LEU:HB2 | 2 | 0.13 |
| (2,1842) | 1:11:A:LEU:HD22 | 1:11:A:LEU:HB2 | 20 | 0.13 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 6 | 0.13 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 7 | 0.13 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 8 | 0.13 |
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 18 | 0.13 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 19 | 0.13 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 3 | 0.13 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 11 | 0.13 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 4 | 0.13 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 7 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 2 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 5 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 7 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 9 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD23 | 1:21:A:LEU:HB3 | 11 | 0.13 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 19 | 0.13 |
| (2,1798) | 1:34:A:VAL:HG22 | 1:74:A:ILE:HD12 | 18 | 0.13 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 3 | 0.13 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 4 | 0.13 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 11 | 0.13 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 12 | 0.13 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 16 | 0.13 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD21 | 18 | 0.13 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 9 | 0.13 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 16 | 0.13 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 20 | 0.13 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 2 | 0.13 |
| (2,1752) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 13 | 0.13 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 5 | 0.13 |
| (2,1745) | 1:34:A:VAL:HA | 1:37:A:LEU:HD21 | 15 | 0.13 |
| (2,1723) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 13 | 0.13 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 1 | 0.13 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 12 | 0.13 |
| (2,1640) | 1:40:A:LYS:HE2 | 1:25:A:ASP:HB2 | 20 | 0.13 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 18 | 0.13 |
| (2,1599) | 1:4:A:MET:HE2 | 1:52:A:GLU:HA | 11 | 0.13 |
| (2,1590) | 1:32:A:ALA:HB2 | 1:33:A:PRO:HD3 | 15 | 0.13 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 7 | 0.13 |
| (2,1511) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 15 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1482) | 1:11:A:LEU:HD12 | 1:11:A:LEU:H | 12 | 0.13 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 19 | 0.13 |
| (2,1455) | 1:165:A:VAL:HG23 | 2:201:A:NAD:H5N | 19 | 0.13 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 2 | 0.13 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 5 | 0.13 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 10 | 0.13 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 16 | 0.13 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 19 | 0.13 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 15 | 0.13 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 1 | 0.13 |
| (2,1279) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 5 | 0.13 |
| (2,1276) | 1:160:A:LEU:HD21 | 1:166:A:TRP:HE1 | 17 | 0.13 |
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 5 | 0.13 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 4 | 0.13 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 20 | 0.13 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 2 | 0.13 |
| (2,1258) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 7 | 0.13 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 2 | 0.13 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 11 | 0.13 |
| (2,1255) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB3 | 12 | 0.13 |
| (2,1158) | 1:165:A:VAL:HG21 | 1:165:A:VAL:H | 15 | 0.13 |
| (2,1110) | 1:76:A:ALA:H | 1:75:A:ARG:H | 16 | 0.13 |
| (2,1099) | 1:100:A:GLY:H | 1:166:A:TRP:H | 7 | 0.13 |
| (2,1071) | 1:86:A:LEU:H | 1:88:A:TYR:H | 9 | 0.13 |
| (2,1026) | 1:84:A:VAL:H | 1:85:A:ASP:H | 5 | 0.13 |
| (2,1025) | 1:84:A:VAL:H | 1:83:A:GLU:H | 3 | 0.13 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 18 | 0.13 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 9 | 0.13 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 11 | 0.13 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 17 | 0.13 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 19 | 0.13 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 11 | 0.13 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 15 | 0.13 |
| (2,948) | 1:76:A:ALA:HB3 | 1:78:A:GLN:HE22 | 14 | 0.13 |
| (2,904) | 1:92:A:VAL:H | 1:92:A:VAL:HA | 13 | 0.13 |
| (2,867) | 1:78:A:GLN:HE22 | 1:76:A:ALA:HA | 3 | 0.13 |
| (2,815) | 1:101:A:THR:HG21 | 1:102:A:ALA:H | 8 | 0.13 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 8 | 0.13 |
| (2,723) | 1:20:A:ALA:HA | 1:23:A:GLY:H | 3 | 0.13 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 8 | 0.13 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 10 | 0.13 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 11 | 0.13 |
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 12 | 0.13 |
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 15 | 0.13 |
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 20 | 0.13 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 7 | 0.13 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 8 | 0.13 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 14 | 0.13 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 16 | 0.13 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 18 | 0.13 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 20 | 0.13 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 10 | 0.13 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 1 | 0.13 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 11 | 0.13 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 12 | 0.13 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 14 | 0.13 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 18 | 0.13 |
| (2,537) | 1:38:A:LEU:H | 1:53:A:LEU:HD11 | 15 | 0.13 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 17 | 0.13 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 4 | 0.13 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 17 | 0.13 |
| (2,431) | 1:73:A:LYS:H | 1:34:A:VAL:HG21 | 4 | 0.13 |
| (2,431) | 1:73:A:LYS:H | 1:34:A:VAL:HG21 | 11 | 0.13 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 17 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 3 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 7 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 9 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 10 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 11 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 13 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 14 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 15 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 17 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 18 | 0.13 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 19 | 0.13 |
| (2,224) | 1:81:A:SER:HA | 1:82:A:VAL:H | 4 | 0.13 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 4 | 0.13 |
| (2,198) | 1:20:A:ALA:HA | 1:24:A:LEU:H | 3 | 0.13 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 4 | 0.13 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 5 | 0.13 |
| (2,196) | 1:24:A:LEU:H | 1:19:A:PRO:HA | 12 | 0.13 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 11 | 0.13 |
| (2,154) | 1:97:A:LEU:H | 1:96:A:VAL:HB | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 3 | 0.13 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 7 | 0.13 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 10 | 0.13 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 11 | 0.13 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 15 | 0.13 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 20 | 0.13 |
| (2,54) | 1:34:A:VAL:H | 1:74:A:ILE:HG22 | 5 | 0.13 |
| (2,54) | 1:34:A:VAL:H | 1:74:A:ILE:HG22 | 15 | 0.13 |
| (2,43) | 1:96:A:VAL:HG21 | 1:148:A:ALA:H | 15 | 0.13 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 20 | 0.13 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 6 | 0.13 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 13 | 0.13 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 8 | 0.13 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 4 | 0.13 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 11 | 0.13 |
| (1,115) | 1:167:A:LEU:H | 1:159:A:TYR:O | 20 | 0.13 |
| (1,104) | 1:147:A:ASP:N | 1:175:A:PHE:O | 8 | 0.13 |
| (1,97) | 1:136:A:MET:H | 1:132:A:ARG:O | 4 | 0.13 |
| (1,91) | 1:133:A:LYS:H | 1:129:A:THR:O | 6 | 0.13 |
| (1,89) | 1:132:A:ARG:H | 1:128:A:ILE:O | 11 | 0.13 |
| (1,88) | 1:131:A:ALA:N | 1:127:A:ASP:O | 14 | 0.13 |
| (1,88) | 1:131:A:ALA:N | 1:127:A:ASP:O | 20 | 0.13 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 8 | 0.13 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 4 | 0.13 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 12 | 0.13 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 17 | 0.13 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 2 | 0.13 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 6 | 0.13 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 11 | 0.13 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 12 | 0.13 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 15 | 0.13 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 12 | 0.13 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 1 | 0.13 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 16 | 0.13 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 2 | 0.13 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 11 | 0.13 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 15 | 0.13 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 5 | 0.13 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 7 | 0.13 |
| (1,24) | 1:37:A:LEU:N | 1:33:A:PRO:O | 1 | 0.13 |
| (1,24) | 1:37:A:LEU:N | 1:33:A:PRO:O | 18 | 0.13 |
| (1,9) | 1:11:A:LEU:H | 1:7:A:VAL:O | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,9) | 1:11:A:LEU:H | 1:7:A:VAL:O | 7 | 0.13 |
| (1,9) | 1:11:A:LEU:H | 1:7:A:VAL:O | 14 | 0.13 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 17 | 0.13 |
| (1,2) | 1:7:A:VAL:N | 1:3:A:HIS:O | 1 | 0.13 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 8 | 0.12 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 13 | 0.12 |
| (4,319) | 1:26:A:LEU:HD21 | 1:14:A:VAL:HA | 16 | 0.12 |
| (4,311) | 1:143:A:VAL:HG13 | 1:178:A:VAL:HA | 1 | 0.12 |
| (4,307) | 1:26:A:LEU:HD22 | 1:15:A:LEU:HA | 3 | 0.12 |
| (4,257) | 1:66:A:ALA:HB2 | 1:66:A:ALA:H | 10 | 0.12 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 2 | 0.12 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 16 | 0.12 |
| (4,209) | 1:76:A:ALA:HB3 | 1:16:A:ARG:H | 10 | 0.12 |
| (4,204) | 1:173:A:ALA:HB3 | 1:111:A:LYS:HG3 | 10 | 0.12 |
| (4,198) | 1:176:A:ILE:HD13 | 1:106:A:PHE:HE1 | 6 | 0.12 |
| (4,198) | 1:176:A:ILE:HD11 | 1:106:A:PHE:HE1 | 18 | 0.12 |
| (4,126) | 1:21:A:LEU:HD13 | 1:14:A:VAL:H | 5 | 0.12 |
| (4,121) | 1:111:A:LYS:H | 1:110:A:LEU:HB2 | 6 | 0.12 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 4 | 0.12 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 11 | 0.12 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 12 | 0.12 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 13 | 0.12 |
| (4,69) | 1:37:A:LEU:H | 1:53:A:LEU:HD11 | 20 | 0.12 |
| (4,65) | 1:6:A:LYS:HB3 | 1:7:A:VAL:H | 14 | 0.12 |
| (4,61) | 1:37:A:LEU:H | 1:38:A:LEU:HD23 | 15 | 0.12 |
| (4,61) | 1:37:A:LEU:H | 1:38:A:LEU:HD23 | 18 | 0.12 |
| (4,41) | 1:5:A:VAL:HG22 | 1:5:A:VAL:H | 3 | 0.12 |
| (4,41) | 1:5:A:VAL:HG21 | 1:5:A:VAL:H | 7 | 0.12 |
| (4,41) | 1:5:A:VAL:HG23 | 1:5:A:VAL:H | 10 | 0.12 |
| (4,41) | 1:5:A:VAL:HG22 | 1:5:A:VAL:H | 17 | 0.12 |
| (4,1) | 1:67:A:PHE:HD1 | 1:37:A:LEU:HD21 | 8 | 0.12 |
| (2,3959) | 1:123:A:HIS:HB3 | 2:201:A:NAD:H5N | 12 | 0.12 |
| (2,3947) | 1:165:A:VAL:HG21 | 2:201:A:NAD:H4N | 15 | 0.12 |
| (2,3940) | 1:134:A:VAL:HG11 | 2:201:A:NAD:H2N | 9 | 0.12 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 4 | 0.12 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 8 | 0.12 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 9 | 0.12 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 10 | 0.12 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 19 | 0.12 |
| (2,3924) | 1:109:A:ILE:HD11 | 2:201:A:NAD:H2A | 3 | 0.12 |
| (2,3924) | 1:109:A:ILE:HD11 | 2:201:A:NAD:H2A | 6 | 0.12 |
| (2,3924) | 1:109:A:ILE:HD11 | 2:201:A:NAD:H2A | 11 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3920) | 1:115:A:LYS:H | 2:201:A:NAD:H8A | 1 | 0.12 |
| (2,3884) | 2:201:A:NAD:H1B | 1:109:A:ILE:HD12 | 20 | 0.12 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 10 | 0.12 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 13 | 0.12 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 18 | 0.12 |
| (2,3861) | 1:24:A:LEU:HG | 1:24:A:LEU:HA | 1 | 0.12 |
| (2,3842) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 4 | 0.12 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 1 | 0.12 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 8 | 0.12 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 9 | 0.12 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 13 | 0.12 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 18 | 0.12 |
| (2,3837) | 1:5:A:VAL:HG23 | 1:5:A:VAL:HA | 8 | 0.12 |
| (2,3825) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB2 | 8 | 0.12 |
| (2,3825) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB2 | 12 | 0.12 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 2 | 0.12 |
| (2,3810) | 1:171:A:VAL:HG22 | 1:168:A:ILE:HD13 | 9 | 0.12 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 8 | 0.12 |
| (2,3802) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 13 | 0.12 |
| (2,3796) | 1:14:A:VAL:HG11 | 1:11:A:LEU:HG | 17 | 0.12 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 19 | 0.12 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 20 | 0.12 |
| (2,3789) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HB3 | 4 | 0.12 |
| (2,3775) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 12 | 0.12 |
| (2,3775) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 17 | 0.12 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 6 | 0.12 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 9 | 0.12 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 11 | 0.12 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 12 | 0.12 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 15 | 0.12 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 18 | 0.12 |
| (2,3770) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 12 | 0.12 |
| (2,3770) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 13 | 0.12 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 9 | 0.12 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 11 | 0.12 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 19 | 0.12 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 4 | 0.12 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 9 | 0.12 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 12 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 2 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 3 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 11 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 12 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 13 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 15 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 16 | 0.12 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 19 | 0.12 |
| (2,3690) | 1:24:A:LEU:HA | 1:24:A:LEU:HD13 | 3 | 0.12 |
| (2,3688) | 1:96:A:VAL:HG11 | 1:94:A:PRO:HA | 18 | 0.12 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 1 | 0.12 |
| (2,3594) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 17 | 0.12 |
| (2,3575) | 1:50:A:MET:HE1 | 1:50:A:MET:HG3 | 1 | 0.12 |
| (2,3575) | 1:50:A:MET:HE1 | 1:50:A:MET:HG3 | 5 | 0.12 |
| (2,3559) | 1:102:A:ALA:HB1 | 2:201:A:NAD:H4B | 3 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HB2 | 1 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 2 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 4 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD13 | 1:53:A:LEU:HB2 | 7 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 9 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD11 | 1:53:A:LEU:HB2 | 11 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 12 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 13 | 0.12 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 15 | 0.12 |
| (2,3518) | 1:128:A:ILE:HD12 | 1:128:A:ILE:HA | 3 | 0.12 |
| (2,3518) | 1:128:A:ILE:HD13 | 1:128:A:ILE:HA | 19 | 0.12 |
| (2,3516) | 1:142:A:VAL:HG12 | 1:109:A:ILE:HA | 19 | 0.12 |
| (2,3500) | 1:144:A:LEU:HD21 | 1:145:A:SER:HB2 | 19 | 0.12 |
| (2,3481) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 15 | 0.12 |
| (2,3481) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 17 | 0.12 |
| (2,3478) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 13 | 0.12 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 3 | 0.12 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 18 | 0.12 |
| (2,3468) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HA | 4 | 0.12 |
| (2,3468) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HA | 7 | 0.12 |
| (2,3467) | 1:11:A:LEU:HD13 | 1:38:A:LEU:HA | 12 | 0.12 |
| (2,3437) | 1:57:A:VAL:HG21 | 1:57:A:VAL:H | 18 | 0.12 |
| (2,3434) | 1:15:A:LEU:HD12 | 1:65:A:PHE:HE1 | 16 | 0.12 |
| (2,3434) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HE1 | 17 | 0.12 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 6 | 0.12 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 11 | 0.12 |
| (2,3382) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HZ | 9 | 0.12 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 6 | 0.12 |
| (2,3379) | 1:66:A:ALA:HB3 | 1:77:A:ASN:HD21 | 16 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 1 | 0.12 |
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 2 | 0.12 |
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 3 | 0.12 |
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 16 | 0.12 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 7 | 0.12 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 13 | 0.12 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 2 | 0.12 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 7 | 0.12 |
| (2,3362) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 3 | 0.12 |
| (2,3362) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 5 | 0.12 |
| (2,3362) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 8 | 0.12 |
| (2,3362) | 1:39:A:ALA:HB3 | 1:40:A:LYS:H | 13 | 0.12 |
| (2,3295) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 12 | 0.12 |
| (2,3295) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 20 | 0.12 |
| (2,3288) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HA | 8 | 0.12 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 2 | 0.12 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 9 | 0.12 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 14 | 0.12 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 17 | 0.12 |
| (2,3257) | 1:117:A:MET:HE2 | 2:201:A:NAD:H2A | 18 | 0.12 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 9 | 0.12 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 10 | 0.12 |
| (2,3253) | 1:160:A:LEU:HD21 | 1:164:A:GLY:HA3 | 15 | 0.12 |
| (2,3232) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HE1 | 8 | 0.12 |
| (2,3230) | 1:176:A:ILE:HD11 | 1:173:A:ALA:HB2 | 4 | 0.12 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 1 | 0.12 |
| (2,3167) | 1:176:A:ILE:HD13 | 1:114:A:ILE:HD13 | 18 | 0.12 |
| (2,3036) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 4 | 0.12 |
| (2,3036) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 15 | 0.12 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 12 | 0.12 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 20 | 0.12 |
| (2,2832) | 1:77:A:ASN:H | 1:77:A:ASN:HD22 | 5 | 0.12 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 19 | 0.12 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 1 | 0.12 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 7 | 0.12 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 12 | 0.12 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 13 | 0.12 |
| (2,2738) | 1:30:A:GLY:H | 1:26:A:LEU:HD21 | 19 | 0.12 |
| (2,2722) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 5 | 0.12 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 6 | 0.12 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 9 | 0.12 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2649) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 5 | 0.12 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 3 | 0.12 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 6 | 0.12 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 10 | 0.12 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 16 | 0.12 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 18 | 0.12 |
| (2,2620) | 1:170:A:PHE:H | 1:168:A:ILE:HG13 | 4 | 0.12 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 12 | 0.12 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 13 | 0.12 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 7 | 0.12 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 10 | 0.12 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 20 | 0.12 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 10 | 0.12 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 11 | 0.12 |
| (2,2566) | 1:43:A:ALA:HB3 | 1:44:A:LYS:H | 20 | 0.12 |
| (2,2520) | 1:8:A:SER:H | 1:6:A:LYS:HA | 16 | 0.12 |
| (2,2492) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 19 | 0.12 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 12 | 0.12 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 14 | 0.12 |
| (2,2254) | 1:6:A:LYS:H | 1:5:A:VAL:HG11 | 8 | 0.12 |
| (2,2234) | 1:14:A:VAL:HG23 | 1:21:A:LEU:H | 6 | 0.12 |
| (2,2212) | 1:53:A:LEU:H | 1:48:A:ILE:HG12 | 8 | 0.12 |
| (2,2210) | 1:48:A:ILE:HD12 | 1:53:A:LEU:H | 10 | 0.12 |
| (2,2210) | 1:48:A:ILE:HD13 | 1:53:A:LEU:H | 20 | 0.12 |
| (2,2192) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 4 | 0.12 |
| (2,2192) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 7 | 0.12 |
| (2,2192) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 14 | 0.12 |
| (2,2189) | 1:81:A:SER:HA | 1:82:A:VAL:H | 4 | 0.12 |
| (2,2175) | 1:57:A:VAL:HG21 | 1:66:A:ALA:H | 2 | 0.12 |
| (2,2175) | 1:57:A:VAL:HG22 | 1:66:A:ALA:H | 10 | 0.12 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD23 | 7 | 0.12 |
| (2,2164) | 1:24:A:LEU:H | 1:24:A:LEU:HB2 | 3 | 0.12 |
| (2,2151) | 1:13:A:LEU:H | 1:13:A:LEU:HB3 | 5 | 0.12 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 13 | 0.12 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 4 | 0.12 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 6 | 0.12 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 7 | 0.12 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 10 | 0.12 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 11 | 0.12 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 18 | 0.12 |
| (2,2132) | 1:56:A:ILE:HD11 | 1:56:A:ILE:H | 10 | 0.12 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 6 | 0.12 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 7 | 0.12 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 9 | 0.12 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 14 | 0.12 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 7 | 0.12 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 11 | 0.12 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 13 | 0.12 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 3 | 0.12 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 6 | 0.12 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 7 | 0.12 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 13 | 0.12 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 18 | 0.12 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 20 | 0.12 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 3 | 0.12 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 4 | 0.12 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 16 | 0.12 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 19 | 0.12 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 14 | 0.12 |
| (2,2010) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 14 | 0.12 |
| (2,1973) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 16 | 0.12 |
| (2,1966) | 1:57:A:VAL:HG12 | 1:67:A:PHE:HE1 | 18 | 0.12 |
| (2,1964) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HD1 | 1 | 0.12 |
| (2,1960) | 1:65:A:PHE:HE1 | 1:15:A:LEU:HD21 | 5 | 0.12 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 4 | 0.12 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 6 | 0.12 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 7 | 0.12 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 8 | 0.12 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 11 | 0.12 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 13 | 0.12 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 14 | 0.12 |
| (2,1924) | 2:201:A:NAD:H51N | 2:201:A:NAD:H52N | 17 | 0.12 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 1 | 0.12 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 4 | 0.12 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 8 | 0.12 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 9 | 0.12 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 12 | 0.12 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 8 | 0.12 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 11 | 0.12 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 16 | 0.12 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 18 | 0.12 |
| (2,1853) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG23 | 18 | 0.12 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1833) | 1:14:A:VAL:HG23 | 1:14:A:VAL:HB | 11 | 0.12 |
| (2,1833) | 1:14:A:VAL:HG21 | 1:14:A:VAL:HB | 12 | 0.12 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 6 | 0.12 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 20 | 0.12 |
| (2,1810) | 1:21:A:LEU:HD12 | 1:21:A:LEU:HB3 | 1 | 0.12 |
| (2,1809) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 10 | 0.12 |
| (2,1809) | 1:34:A:VAL:HG13 | 1:37:A:LEU:HB3 | 18 | 0.12 |
| (2,1805) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 8 | 0.12 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 10 | 0.12 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 7 | 0.12 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 9 | 0.12 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 13 | 0.12 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 19 | 0.12 |
| (2,1729) | 1:41:A:MET:HA | 1:22:A:ILE:HB | 7 | 0.12 |
| (2,1723) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 7 | 0.12 |
| (2,1723) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 20 | 0.12 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 6 | 0.12 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 13 | 0.12 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 17 | 0.12 |
| (2,1687) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 5 | 0.12 |
| (2,1601) | 1:41:A:MET:HE3 | 1:10:A:PHE:HB3 | 14 | 0.12 |
| (2,1599) | 1:4:A:MET:HE3 | 1:52:A:GLU:HA | 16 | 0.12 |
| (2,1590) | 1:32:A:ALA:HB2 | 1:33:A:PRO:HD3 | 2 | 0.12 |
| (2,1588) | 1:152:A:ALA:HB2 | 1:149:A:LYS:HA | 19 | 0.12 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 10 | 0.12 |
| (2,1511) | 1:82:A:VAL:HG21 | 1:80:A:HIS:HA | 17 | 0.12 |
| (2,1509) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 10 | 0.12 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 18 | 0.12 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 14 | 0.12 |
| (2,1440) | 1:37:A:LEU:HD12 | 1:37:A:LEU:H | 2 | 0.12 |
| (2,1440) | 1:37:A:LEU:HD11 | 1:37:A:LEU:H | 4 | 0.12 |
| (2,1440) | 1:37:A:LEU:HD11 | 1:37:A:LEU:H | 5 | 0.12 |
| (2,1440) | 1:37:A:LEU:HD12 | 1:37:A:LEU:H | 18 | 0.12 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 12 | 0.12 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 16 | 0.12 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 18 | 0.12 |
| (2,1432) | 1:38:A:LEU:HD12 | 1:39:A:ALA:H | 3 | 0.12 |
| (2,1432) | 1:38:A:LEU:HD11 | 1:39:A:ALA:H | 11 | 0.12 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 7 | 0.12 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 1 | 0.12 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 9 | 0.12 |
| (2,1308) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HA | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 12 | 0.12 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 16 | 0.12 |
| (2,1259) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 5 | 0.12 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 18 | 0.12 |
| (2,1219) | 1:177:A:LYS:HA | 1:178:A:VAL:HG21 | 2 | 0.12 |
| (2,1208) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 20 | 0.12 |
| (2,1207) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 9 | 0.12 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 7 | 0.12 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 11 | 0.12 |
| (2,1110) | 1:76:A:ALA:H | 1:75:A:ARG:H | 8 | 0.12 |
| (2,1099) | 1:100:A:GLY:H | 1:166:A:TRP:H | 14 | 0.12 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 8 | 0.12 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 1 | 0.12 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 9 | 0.12 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 15 | 0.12 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 16 | 0.12 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 18 | 0.12 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 19 | 0.12 |
| (2,1001) | 1:177:A:LYS:H | 1:145:A:SER:H | 9 | 0.12 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 12 | 0.12 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 16 | 0.12 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 5 | 0.12 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 9 | 0.12 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 19 | 0.12 |
| (2,904) | 1:92:A:VAL:H | 1:92:A:VAL:HA | 5 | 0.12 |
| (2,904) | 1:92:A:VAL:H | 1:92:A:VAL:HA | 14 | 0.12 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 4 | 0.12 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 6 | 0.12 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 14 | 0.12 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 19 | 0.12 |
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 4 | 0.12 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 4 | 0.12 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 11 | 0.12 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 19 | 0.12 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 20 | 0.12 |
| (2,639) | 1:173:A:ALA:HB1 | 1:174:A:GLU:H | 15 | 0.12 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 6 | 0.12 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 2 | 0.12 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 4 | 0.12 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 6 | 0.12 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 9 | 0.12 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 15 | 0.12 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 3 | 0.12 |
| (2,458) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 7 | 0.12 |
| (2,453) | 1:34:A:VAL:HB | 1:35:A:LYS:H | 12 | 0.12 |
| (2,431) | 1:73:A:LYS:H | 1:34:A:VAL:HG21 | 13 | 0.12 |
| (2,409) | 1:11:A:LEU:H | 1:11:A:LEU:HG | 5 | 0.12 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 9 | 0.12 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 4 | 0.12 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 20 | 0.12 |
| (2,303) | 1:84:A:VAL:H | 1:83:A:GLU:HB3 | 17 | 0.12 |
| (2,300) | 1:153:A:ASP:H | 1:95:A:ALA:HB1 | 11 | 0.12 |
| (2,268) | 1:14:A:VAL:HG21 | 1:21:A:LEU:H | 15 | 0.12 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 10 | 0.12 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 17 | 0.12 |
| (2,212) | 1:74:A:ILE:HD11 | 1:75:A:ARG:H | 19 | 0.12 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 1 | 0.12 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 3 | 0.12 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 9 | 0.12 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 13 | 0.12 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 14 | 0.12 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 20 | 0.12 |
| (2,184) | 1:26:A:LEU:H | 1:19:A:PRO:HA | 15 | 0.12 |
| (2,171) | 1:56:A:ILE:H | 1:55:A:HIS:HB3 | 3 | 0.12 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 7 | 0.12 |
| (2,161) | 1:86:A:LEU:HA | 1:86:A:LEU:H | 17 | 0.12 |
| (2,144) | 1:82:A:VAL:HB | 1:83:A:GLU:H | 17 | 0.12 |
| (2,142) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 18 | 0.12 |
| (2,127) | 1:92:A:VAL:H | 1:91:A:GLN:HG3 | 1 | 0.12 |
| (2,121) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 11 | 0.12 |
| (2,99) | 1:140:A:LYS:H | 1:103:A:GLU:HA | 3 | 0.12 |
| (2,96) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 5 | 0.12 |
| (2,85) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H | 2 | 0.12 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 6 | 0.12 |
| (2,43) | 1:96:A:VAL:HG21 | 1:148:A:ALA:H | 11 | 0.12 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 2 | 0.12 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 6 | 0.12 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 14 | 0.12 |
| (1,126) | 1:177:A:LYS:N | 1:145:A:SER:O | 15 | 0.12 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 1 | 0.12 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 17 | 0.12 |
| (1,122) | 1:175:A:PHE:N | 1:172:A:PRO:O | 20 | 0.12 |
| (1,121) | 1:175:A:PHE:H | 1:172:A:PRO:O | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,121) | 1:175:A:PHE:H | 1:172:A:PRO:O | 3 | 0.12 |
| (1,119) | 1:171:A:VAL:H | 1:114:A:ILE:O | 14 | 0.12 |
| (1,110) | 1:153:A:ASP:N | 1:149:A:LYS:O | 9 | 0.12 |
| (1,110) | 1:153:A:ASP:N | 1:149:A:LYS:O | 10 | 0.12 |
| (1,106) | 1:150:A:GLY:N | 1:147:A:ASP:O | 11 | 0.12 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 18 | 0.12 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 20 | 0.12 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 9 | 0.12 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 13 | 0.12 |
| (1,97) | 1:136:A:MET:H | 1:132:A:ARG:O | 5 | 0.12 |
| (1,97) | 1:136:A:MET:H | 1:132:A:ARG:O | 14 | 0.12 |
| (1,94) | 1:134:A:VAL:N | 1:130:A:THR:O | 18 | 0.12 |
| (1,92) | 1:133:A:LYS:N | 1:129:A:THR:O | 8 | 0.12 |
| (1,92) | 1:133:A:LYS:N | 1:129:A:THR:O | 12 | 0.12 |
| (1,91) | 1:133:A:LYS:H | 1:129:A:THR:O | 2 | 0.12 |
| (1,91) | 1:133:A:LYS:H | 1:129:A:THR:O | 9 | 0.12 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 4 | 0.12 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 5 | 0.12 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 7 | 0.12 |
| (1,88) | 1:131:A:ALA:N | 1:127:A:ASP:O | 6 | 0.12 |
| (1,86) | 1:124:A:LEU:N | 1:166:A:TRP:O | 18 | 0.12 |
| (1,85) | 1:124:A:LEU:H | 1:166:A:TRP:O | 5 | 0.12 |
| (1,82) | 1:114:A:ILE:N | 1:171:A:VAL:O | 9 | 0.12 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 3 | 0.12 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 19 | 0.12 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 8 | 0.12 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 14 | 0.12 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 16 | 0.12 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 16 | 0.12 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 8 | 0.12 |
| (1,56) | 1:74:A:ILE:N | 1:32:A:ALA:O | 4 | 0.12 |
| (1,55) | 1:74:A:ILE:H | 1:32:A:ALA:O | 1 | 0.12 |
| (1,55) | 1:74:A:ILE:H | 1:32:A:ALA:O | 8 | 0.12 |
| (1,48) | 1:58:A:GLU:N | 1:54:A:LYS:O | 3 | 0.12 |
| (1,45) | 1:57:A:VAL:H | 1:53:A:LEU:O | 2 | 0.12 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 9 | 0.12 |
| (1,39) | 1:54:A:LYS:H | 1:50:A:MET:O | 8 | 0.12 |
| (1,39) | 1:54:A:LYS:H | 1:50:A:MET:O | 10 | 0.12 |
| (1,39) | 1:54:A:LYS:H | 1:50:A:MET:O | 19 | 0.12 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 4 | 0.12 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 6 | 0.12 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 9 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 13 | 0.12 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 14 | 0.12 |
| (1,21) | 1:32:A:ALA:H | 1:74:A:ILE:O | 5 | 0.12 |
| (1,15) | 1:14:A:VAL:H | 1:10:A:PHE:O | 5 | 0.12 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 20 | 0.12 |
| (4,442) | 1:178:A:VAL:HG21 | 1:144:A:LEU:HG | 5 | 0.11 |
| (4,425) | 1:34:A:VAL:HG21 | 1:35:A:LYS:HB2 | 8 | 0.11 |
| (4,385) | 1:15:A:LEU:HA | 1:14:A:VAL:HG11 | 1 | 0.11 |
| (4,379) | 1:50:A:MET:HA | 1:35:A:LYS:HG2 | 14 | 0.11 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 1 | 0.11 |
| (4,328) | 1:122:A:VAL:HG13 | 1:113:A:GLY:HA2 | 1 | 0.11 |
| (4,311) | 1:143:A:VAL:HG12 | 1:178:A:VAL:HA | 19 | 0.11 |
| (4,303) | 1:110:A:LEU:HD11 | 1:107:A:ASP:HA | 19 | 0.11 |
| (4,297) | 1:168:A:ILE:HD13 | 1:114:A:ILE:H | 17 | 0.11 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HZ | 2 | 0.11 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HZ | 18 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 3 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 7 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 9 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 10 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 11 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 13 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 14 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 15 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 17 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 18 | 0.11 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 19 | 0.11 |
| (4,213) | 1:165:A:VAL:HB | 1:123:A:HIS:HA | 2 | 0.11 |
| (4,198) | 1:176:A:ILE:HD11 | 1:106:A:PHE:HE1 | 7 | 0.11 |
| (4,198) | 1:176:A:ILE:HD11 | 1:106:A:PHE:HE1 | 14 | 0.11 |
| (4,198) | 1:176:A:ILE:HD11 | 1:106:A:PHE:HE1 | 19 | 0.11 |
| (4,166) | 1:171:A:VAL:H | 1:124:A:LEU:HD11 | 15 | 0.11 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 2 | 0.11 |
| (4,69) | 1:57:A:VAL:H | 1:56:A:ILE:HG12 | 6 | 0.11 |
| (4,65) | 1:6:A:LYS:HB3 | 1:7:A:VAL:H | 3 | 0.11 |
| (4,65) | 1:7:A:VAL:H | 1:7:A:VAL:HB | 9 | 0.11 |
| (4,61) | 1:37:A:LEU:H | 1:38:A:LEU:HD23 | 10 | 0.11 |
| (4,61) | 1:37:A:LEU:H | 1:38:A:LEU:HD23 | 20 | 0.11 |
| (4,41) | 1:5:A:VAL:HG23 | 1:5:A:VAL:H | 2 | 0.11 |
| (4,41) | 1:5:A:VAL:HG22 | 1:5:A:VAL:H | 4 | 0.11 |
| (4,41) | 1:5:A:VAL:HG23 | 1:5:A:VAL:H | 5 | 0.11 |
| (4,41) | 1:5:A:VAL:HG23 | 1:5:A:VAL:H | 11 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (4,41) | 1:5:A:VAL:HG22 | 1:5:A:VAL:H | 13 | 0.11 |
| (4,41) | 1:5:A:VAL:HG21 | 1:5:A:VAL:H | 14 | 0.11 |
| (4,41) | 1:5:A:VAL:HG21 | 1:5:A:VAL:H | 15 | 0.11 |
| (4,23) | 1:39:A:ALA:H | 1:42:A:LYS:HB2 | 7 | 0.11 |
| (4,8) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HD1 | 2 | 0.11 |
| (4,8) | 1:22:A:ILE:HG23 | 1:10:A:PHE:HD1 | 6 | 0.11 |
| (2,3952) | 1:165:A:VAL:HG11 | 2:201:A:NAD:H5N | 18 | 0.11 |
| (2,3935) | 1:102:A:ALA:HB1 | 2:201:A:NAD:HO3A | 18 | 0.11 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 3 | 0.11 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 4 | 0.11 |
| (2,3903) | 2:201:A:NAD:H6N | 1:165:A:VAL:HG12 | 19 | 0.11 |
| (2,3898) | 2:201:A:NAD:H1D | 2:201:A:NAD:H6N | 4 | 0.11 |
| (2,3884) | 2:201:A:NAD:H1B | 1:109:A:ILE:HD12 | 9 | 0.11 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 2 | 0.11 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 6 | 0.11 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 11 | 0.11 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 15 | 0.11 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 4 | 0.11 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 5 | 0.11 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 10 | 0.11 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 11 | 0.11 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 12 | 0.11 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 17 | 0.11 |
| (2,3829) | 1:109:A:ILE:HD11 | 1:101:A:THR:HG23 | 4 | 0.11 |
| (2,3820) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HD11 | 1 | 0.11 |
| (2,3820) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HD11 | 10 | 0.11 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 12 | 0.11 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 14 | 0.11 |
| (2,3820) | 1:109:A:ILE:HG23 | 1:109:A:ILE:HD11 | 19 | 0.11 |
| (2,3815) | 1:21:A:LEU:HD13 | 1:14:A:VAL:HG22 | 20 | 0.11 |
| (2,3812) | 1:56:A:ILE:HG23 | 1:11:A:LEU:HD11 | 17 | 0.11 |
| (2,3802) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 1 | 0.11 |
| (2,3802) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3 | 3 | 0.11 |
| (2,3802) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3 | 7 | 0.11 |
| (2,3802) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3 | 11 | 0.11 |
| (2,3796) | 1:14:A:VAL:HG12 | 1:11:A:LEU:HG | 12 | 0.11 |
| (2,3785) | 1:142:A:VAL:HG11 | 1:103:A:GLU:HG2 | 17 | 0.11 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 10 | 0.11 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 13 | 0.11 |
| (2,3775) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 2 | 0.11 |
| (2,3775) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 14 | 0.11 |
| (2,3775) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 16 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 7 | 0.11 |
| (2,3773) | 1:34:A:VAL:HG11 | 1:37:A:LEU:HB3 | 13 | 0.11 |
| (2,3764) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 14 | 0.11 |
| (2,3764) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 17 | 0.11 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 4 | 0.11 |
| (2,3763) | 1:76:A:ALA:HB3 | 1:15:A:LEU:HD11 | 19 | 0.11 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 2 | 0.11 |
| (2,3726) | 1:44:A:LYS:HE2 | 1:22:A:ILE:HG22 | 18 | 0.11 |
| (2,3722) | 1:16:A:ARG:HD3 | 1:76:A:ALA:HB1 | 1 | 0.11 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 1 | 0.11 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 3 | 0.11 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 5 | 0.11 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 10 | 0.11 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 20 | 0.11 |
| (2,3712) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 10 | 0.11 |
| (2,3712) | 1:109:A:ILE:HG22 | 1:109:A:ILE:HA | 12 | 0.11 |
| (2,3712) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 19 | 0.11 |
| (2,3712) | 1:109:A:ILE:HG21 | 1:109:A:ILE:HA | 20 | 0.11 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 6 | 0.11 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 7 | 0.11 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 9 | 0.11 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 10 | 0.11 |
| (2,3708) | 1:173:A:ALA:HA | 1:176:A:ILE:HD11 | 18 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 2 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 5 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 6 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 8 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 9 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 11 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 12 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 13 | 0.11 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 16 | 0.11 |
| (2,3679) | 1:97:A:LEU:HD21 | 1:97:A:LEU:HA | 17 | 0.11 |
| (2,3575) | 1:50:A:MET:HE3 | 1:50:A:MET:HG3 | 20 | 0.11 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 2 | 0.11 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 10 | 0.11 |
| (2,3514) | 1:143:A:VAL:HG12 | 1:132:A:ARG:HA | 1 | 0.11 |
| (2,3509) | 1:13:A:LEU:HD23 | 1:17:A:HIS:HB2 | 11 | 0.11 |
| (2,3479) | 1:151:A:MET:HE1 | 1:171:A:VAL:HA | 5 | 0.11 |
| (2,3479) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 16 | 0.11 |
| (2,3479) | 1:151:A:MET:HE3 | 1:171:A:VAL:HA | 19 | 0.11 |
| (2,3478) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3478) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 20 | 0.11 |
| (2,3473) | 1:146:A:VAL:HG22 | 1:96:A:VAL:HA | 13 | 0.11 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 15 | 0.11 |
| (2,3473) | 1:146:A:VAL:HG21 | 1:96:A:VAL:HA | 17 | 0.11 |
| (2,3473) | 1:146:A:VAL:HG23 | 1:96:A:VAL:HA | 20 | 0.11 |
| (2,3468) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HA | 3 | 0.11 |
| (2,3468) | 1:110:A:LEU:HD12 | 1:110:A:LEU:HA | 17 | 0.11 |
| (2,3446) | 1:74:A:ILE:HD12 | 1:67:A:PHE:HE1 | 15 | 0.11 |
| (2,3414) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 9 | 0.11 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 2 | 0.11 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 3 | 0.11 |
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 9 | 0.11 |
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 18 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 2 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 3 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 8 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 9 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 12 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 14 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 15 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 16 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 19 | 0.11 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 20 | 0.11 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 14 | 0.11 |
| (2,3362) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 9 | 0.11 |
| (2,3362) | 1:39:A:ALA:HB2 | 1:40:A:LYS:H | 19 | 0.11 |
| (2,3345) | 1:41:A:MET:HE2 | 1:10:A:PHE:HE1 | 16 | 0.11 |
| (2,3335) | 1:16:A:ARG:HD2 | 1:12:A:SER:H | 17 | 0.11 |
| (2,3302) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 2 | 0.11 |
| (2,3295) | 1:50:A:MET:HA | 1:70:A:ASN:HD22 | 3 | 0.11 |
| (2,3288) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 2 | 0.11 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 1 | 0.11 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 4 | 0.11 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 7 | 0.11 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 8 | 0.11 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 13 | 0.11 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 19 | 0.11 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 20 | 0.11 |
| (2,3266) | 1:53:A:LEU:HD13 | 1:67:A:PHE:HE1 | 9 | 0.11 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 3 | 0.11 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 8 | 0.11 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 11 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 12 | 0.11 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 15 | 0.11 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 19 | 0.11 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 6 | 0.11 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 7 | 0.11 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 11 | 0.11 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 12 | 0.11 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 13 | 0.11 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 14 | 0.11 |
| (2,3233) | 1:171:A:VAL:HG11 | 1:171:A:VAL:H | 5 | 0.11 |
| (2,3231) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 10 | 0.11 |
| (2,3197) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 16 | 0.11 |
| (2,3184) | 1:92:A:VAL:HG21 | 1:92:A:VAL:H | 20 | 0.11 |
| (2,3182) | 1:114:A:ILE:HD13 | 1:171:A:VAL:HB | 2 | 0.11 |
| (2,3180) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 3 | 0.11 |
| (2,3180) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 10 | 0.11 |
| (2,3180) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 13 | 0.11 |
| (2,3180) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 20 | 0.11 |
| (2,3173) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 9 | 0.11 |
| (2,3173) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 11 | 0.11 |
| (2,3173) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 14 | 0.11 |
| (2,3127) | 1:97:A:LEU:HD11 | 1:124:A:LEU:HD23 | 2 | 0.11 |
| (2,3102) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 18 | 0.11 |
| (2,3102) | 1:136:A:MET:H | 1:105:A:ASN:HD22 | 19 | 0.11 |
| (2,3036) | 1:161:A:SER:H | 2:201:A:NAD:H6N | 6 | 0.11 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 2 | 0.11 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 4 | 0.11 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 13 | 0.11 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 17 | 0.11 |
| (2,2980) | 1:40:A:LYS:H | 1:39:A:ALA:H | 1 | 0.11 |
| (2,2980) | 1:40:A:LYS:H | 1:39:A:ALA:H | 4 | 0.11 |
| (2,2980) | 1:40:A:LYS:H | 1:39:A:ALA:H | 17 | 0.11 |
| (2,2887) | 1:176:A:ILE:H | 1:146:A:VAL:HG11 | 2 | 0.11 |
| (2,2887) | 1:176:A:ILE:H | 1:146:A:VAL:HG11 | 11 | 0.11 |
| (2,2887) | 1:176:A:ILE:H | 1:146:A:VAL:HG11 | 15 | 0.11 |
| (2,2887) | 1:176:A:ILE:H | 1:146:A:VAL:HG11 | 16 | 0.11 |
| (2,2841) | 1:78:A:GLN:HE22 | 1:77:A:ASN:H | 11 | 0.11 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 15 | 0.11 |
| (2,2757) | 1:59:A:THR:H | 1:76:A:ALA:HA | 17 | 0.11 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 3 | 0.11 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 5 | 0.11 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 17 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 19 | 0.11 |
| (2,2722) | 1:139:A:GLY:H | 1:103:A:GLU:HA | 4 | 0.11 |
| (2,2680) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 3 | 0.11 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 2 | 0.11 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 7 | 0.11 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 13 | 0.11 |
| (2,2649) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 4 | 0.11 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB1 | 13 | 0.11 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 14 | 0.11 |
| (2,2632) | 1:29:A:ASN:H | 1:28:A:ALA:HB3 | 17 | 0.11 |
| (2,2627) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 6 | 0.11 |
| (2,2597) | 1:44:A:LYS:H | 1:21:A:LEU:HA | 6 | 0.11 |
| (2,2597) | 1:44:A:LYS:H | 1:21:A:LEU:HA | 19 | 0.11 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 6 | 0.11 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 18 | 0.11 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 3 | 0.11 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 15 | 0.11 |
| (2,2574) | 1:111:A:LYS:HB3 | 1:111:A:LYS:H | 2 | 0.11 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 6 | 0.11 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 8 | 0.11 |
| (2,2566) | 1:43:A:ALA:HB2 | 1:44:A:LYS:H | 9 | 0.11 |
| (2,2550) | 1:86:A:LEU:H | 1:88:A:TYR:H | 4 | 0.11 |
| (2,2526) | 1:7:A:VAL:HG11 | 1:8:A:SER:H | 20 | 0.11 |
| (2,2492) | 1:129:A:THR:HG22 | 1:129:A:THR:H | 11 | 0.11 |
| (2,2429) | 1:35:A:LYS:H | 1:34:A:VAL:HG12 | 20 | 0.11 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 3 | 0.11 |
| (2,2401) | 1:73:A:LYS:H | 1:73:A:LYS:HB3 | 7 | 0.11 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 19 | 0.11 |
| (2,2308) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 6 | 0.11 |
| (2,2305) | 1:173:A:ALA:HB1 | 1:176:A:ILE:H | 4 | 0.11 |
| (2,2305) | 1:173:A:ALA:HB1 | 1:176:A:ILE:H | 14 | 0.11 |
| (2,2269) | 1:84:A:VAL:HA | 1:84:A:VAL:H | 5 | 0.11 |
| (2,2269) | 1:84:A:VAL:HA | 1:84:A:VAL:H | 17 | 0.11 |
| (2,2216) | 1:26:A:LEU:HD13 | 1:27:A:ASP:H | 7 | 0.11 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 9 | 0.11 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 10 | 0.11 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 14 | 0.11 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 15 | 0.11 |
| (2,2192) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 13 | 0.11 |
| (2,2189) | 1:81:A:SER:HA | 1:82:A:VAL:H | 14 | 0.11 |
| (2,2166) | 1:24:A:LEU:H | 1:24:A:LEU:HD21 | 11 | 0.11 |
| (2,2148) | 1:26:A:LEU:HD21 | 1:26:A:LEU:H | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 13 | 0.11 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 14 | 0.11 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 2 | 0.11 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 3 | 0.11 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 4 | 0.11 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 11 | 0.11 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 15 | 0.11 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 16 | 0.11 |
| (2,2130) | 1:56:A:ILE:H | 1:56:A:ILE:HB | 20 | 0.11 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 5 | 0.11 |
| (2,2122) | 1:86:A:LEU:HB2 | 1:86:A:LEU:H | 11 | 0.11 |
| (2,2098) | 1:83:A:GLU:HB2 | 1:83:A:GLU:H | 17 | 0.11 |
| (2,2090) | 1:32:A:ALA:H | 1:26:A:LEU:HD13 | 7 | 0.11 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 4 | 0.11 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 17 | 0.11 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 4 | 0.11 |
| (2,2075) | 1:178:A:VAL:H | 1:177:A:LYS:H | 17 | 0.11 |
| (2,2067) | 1:91:A:GLN:H | 1:159:A:TYR:HD1 | 15 | 0.11 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 10 | 0.11 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 12 | 0.11 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 7 | 0.11 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 9 | 0.11 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 13 | 0.11 |
| (2,2047) | 1:25:A:ASP:H | 1:26:A:LEU:HG | 18 | 0.11 |
| (2,2018) | 1:166:A:TRP:HE1 | 1:126:A:GLN:HB2 | 6 | 0.11 |
| (2,2010) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 2 | 0.11 |
| (2,2010) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 4 | 0.11 |
| (2,2010) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 15 | 0.11 |
| (2,1989) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 8 | 0.11 |
| (2,1989) | 1:142:A:VAL:HG21 | 1:106:A:PHE:HD1 | 15 | 0.11 |
| (2,1964) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HD1 | 11 | 0.11 |
| (2,1964) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HD1 | 20 | 0.11 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 3 | 0.11 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 5 | 0.11 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 10 | 0.11 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG23 | 11 | 0.11 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 17 | 0.11 |
| (2,1876) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 19 | 0.11 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 20 | 0.11 |
| (2,1863) | 1:11:A:LEU:HD11 | 1:11:A:LEU:HB3 | 20 | 0.11 |
| (2,1860) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 6 | 0.11 |
| (2,1860) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1860) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 14 | 0.11 |
| (2,1860) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB | 16 | 0.11 |
| (2,1852) | 1:57:A:VAL:HG12 | 1:74:A:ILE:HD13 | 8 | 0.11 |
| (2,1849) | 1:15:A:LEU:HD12 | 1:74:A:ILE:HD12 | 20 | 0.11 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 4 | 0.11 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 9 | 0.11 |
| (2,1810) | 1:21:A:LEU:HD12 | 1:21:A:LEU:HB3 | 3 | 0.11 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 14 | 0.11 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 16 | 0.11 |
| (2,1805) | 1:21:A:LEU:HD21 | 1:21:A:LEU:HB3 | 17 | 0.11 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 2 | 0.11 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD12 | 6 | 0.11 |
| (2,1797) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 19 | 0.11 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 1 | 0.11 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 3 | 0.11 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 4 | 0.11 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 15 | 0.11 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 17 | 0.11 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 1 | 0.11 |
| (2,1746) | 1:32:A:ALA:HB1 | 1:33:A:PRO:HD3 | 3 | 0.11 |
| (2,1733) | 1:7:A:VAL:HA | 1:7:A:VAL:HB | 12 | 0.11 |
| (2,1723) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 3 | 0.11 |
| (2,1723) | 1:38:A:LEU:HD13 | 1:50:A:MET:HA | 8 | 0.11 |
| (2,1723) | 1:38:A:LEU:HD11 | 1:50:A:MET:HA | 18 | 0.11 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 15 | 0.11 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 16 | 0.11 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 20 | 0.11 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 1 | 0.11 |
| (2,1625) | 1:52:A:GLU:HG2 | 1:47:A:GLY:HA2 | 17 | 0.11 |
| (2,1603) | 1:71:A:PHE:HB3 | 1:50:A:MET:HE3 | 19 | 0.11 |
| (2,1591) | 1:95:A:ALA:HB1 | 1:149:A:LYS:HA | 15 | 0.11 |
| (2,1563) | 1:48:A:ILE:HG23 | 1:53:A:LEU:HB2 | 11 | 0.11 |
| (2,1549) | 1:37:A:LEU:HD13 | 1:41:A:MET:HG2 | 18 | 0.11 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 5 | 0.11 |
| (2,1540) | 1:56:A:ILE:HG21 | 1:56:A:ILE:HA | 17 | 0.11 |
| (2,1474) | 1:110:A:LEU:HD21 | 1:110:A:LEU:H | 9 | 0.11 |
| (2,1474) | 1:110:A:LEU:HD21 | 1:110:A:LEU:H | 12 | 0.11 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 4 | 0.11 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 11 | 0.11 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 12 | 0.11 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 19 | 0.11 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1440) | 1:37:A:LEU:HD12 | 1:37:A:LEU:H | 3 | 0.11 |
| (2,1440) | 1:37:A:LEU:HD12 | 1:37:A:LEU:H | 6 | 0.11 |
| (2,1440) | 1:37:A:LEU:HD12 | 1:37:A:LEU:H | 7 | 0.11 |
| (2,1440) | 1:37:A:LEU:HD13 | 1:37:A:LEU:H | 8 | 0.11 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 6 | 0.11 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 9 | 0.11 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 11 | 0.11 |
| (2,1424) | 1:56:A:ILE:HG22 | 1:65:A:PHE:HE1 | 16 | 0.11 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 3 | 0.11 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 5 | 0.11 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 8 | 0.11 |
| (2,1348) | 1:83:A:GLU:HA | 1:84:A:VAL:H | 14 | 0.11 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 15 | 0.11 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 17 | 0.11 |
| (2,1314) | 1:142:A:VAL:HG13 | 1:103:A:GLU:HA | 13 | 0.11 |
| (2,1308) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HA | 17 | 0.11 |
| (2,1308) | 1:13:A:LEU:HD11 | 1:13:A:LEU:HA | 20 | 0.11 |
| (2,1275) | 1:160:A:LEU:HD21 | 1:161:A:SER:H | 12 | 0.11 |
| (2,1256) | 1:173:A:ALA:HB3 | 1:110:A:LEU:HD12 | 2 | 0.11 |
| (2,1206) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 18 | 0.11 |
| (2,1203) | 1:24:A:LEU:HD13 | 1:36:A:GLU:HG3 | 1 | 0.11 |
| (2,1172) | 1:144:A:LEU:HD11 | 1:106:A:PHE:HE1 | 19 | 0.11 |
| (2,1080) | 1:21:A:LEU:H | 1:22:A:ILE:H | 5 | 0.11 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 5 | 0.11 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 12 | 0.11 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 15 | 0.11 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 16 | 0.11 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 6 | 0.11 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 11 | 0.11 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 14 | 0.11 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 6 | 0.11 |
| (2,979) | 1:96:A:VAL:H | 1:95:A:ALA:H | 7 | 0.11 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 2 | 0.11 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 8 | 0.11 |
| (2,950) | 1:76:A:ALA:H | 1:76:A:ALA:HA | 2 | 0.11 |
| (2,950) | 1:76:A:ALA:H | 1:76:A:ALA:HA | 14 | 0.11 |
| (2,950) | 1:76:A:ALA:H | 1:76:A:ALA:HA | 18 | 0.11 |
| (2,942) | 1:114:A:ILE:H | 1:170:A:PHE:HD1 | 2 | 0.11 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 2 | 0.11 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 17 | 0.11 |
| (2,693) | 1:126:A:GLN:HE22 | 1:166:A:TRP:HB2 | 2 | 0.11 |
| (2,676) | 1:70:A:ASN:HD22 | 1:50:A:MET:HB2 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,660) | 1:29:A:ASN:H | 1:28:A:ALA:HB2 | 15 | 0.11 |
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 8 | 0.11 |
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 19 | 0.11 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 17 | 0.11 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 8 | 0.11 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 11 | 0.11 |
| (2,628) | 1:44:A:LYS:HB3 | 1:44:A:LYS:H | 17 | 0.11 |
| (2,550) | 1:102:A:ALA:HB1 | 1:105:A:ASN:H | 12 | 0.11 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 5 | 0.11 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 8 | 0.11 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 17 | 0.11 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 19 | 0.11 |
| (2,538) | 1:38:A:LEU:HA | 1:38:A:LEU:H | 20 | 0.11 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 4 | 0.11 |
| (2,473) | 1:110:A:LEU:H | 1:110:A:LEU:HB3 | 16 | 0.11 |
| (2,468) | 1:51:A:GLU:H | 1:50:A:MET:HB2 | 19 | 0.11 |
| (2,445) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 4 | 0.11 |
| (2,439) | 1:55:A:HIS:H | 1:54:A:LYS:HB2 | 4 | 0.11 |
| (2,413) | 1:11:A:LEU:H | 1:11:A:LEU:HA | 5 | 0.11 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 3 | 0.11 |
| (2,382) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 1 | 0.11 |
| (2,342) | 1:41:A:MET:H | 1:41:A:MET:HG2 | 20 | 0.11 |
| (2,268) | 1:14:A:VAL:HG21 | 1:21:A:LEU:H | 2 | 0.11 |
| (2,268) | 1:14:A:VAL:HG22 | 1:21:A:LEU:H | 8 | 0.11 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 4 | 0.11 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 5 | 0.11 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 7 | 0.11 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 3 | 0.11 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 5 | 0.11 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 6 | 0.11 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 11 | 0.11 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 12 | 0.11 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 19 | 0.11 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 20 | 0.11 |
| (2,224) | 1:81:A:SER:HA | 1:82:A:VAL:H | 14 | 0.11 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 10 | 0.11 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 15 | 0.11 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 16 | 0.11 |
| (2,148) | 1:85:A:ASP:H | 1:85:A:ASP:HB3 | 20 | 0.11 |
| (2,99) | 1:140:A:LYS:H | 1:103:A:GLU:HA | 2 | 0.11 |
| (2,85) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H | 4 | 0.11 |
| (2,65) | 1:177:A:LYS:H | 1:177:A:LYS:HD2 | 19 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,62) | 1:178:A:VAL:H | 1:177:A:LYS:H | 5 | 0.11 |
| (2,62) | 1:178:A:VAL:H | 1:177:A:LYS:H | 9 | 0.11 |
| (2,62) | 1:178:A:VAL:H | 1:177:A:LYS:H | 12 | 0.11 |
| (2,62) | 1:178:A:VAL:H | 1:177:A:LYS:H | 16 | 0.11 |
| (2,61) | 1:166:A:TRP:HE1 | 1:126:A:GLN:HB2 | 14 | 0.11 |
| (2,54) | 1:34:A:VAL:H | 1:74:A:ILE:HG21 | 12 | 0.11 |
| (2,42) | 1:148:A:ALA:H | 1:148:A:ALA:HB1 | 5 | 0.11 |
| (2,42) | 1:148:A:ALA:H | 1:148:A:ALA:HB1 | 9 | 0.11 |
| (2,42) | 1:148:A:ALA:H | 1:148:A:ALA:HB1 | 19 | 0.11 |
| (2,42) | 1:148:A:ALA:H | 1:148:A:ALA:HB1 | 20 | 0.11 |
| (2,20) | 1:3:A:HIS:HD2 | 1:3:A:HIS:HB2 | 13 | 0.11 |
| (2,14) | 1:34:A:VAL:HG23 | 1:67:A:PHE:HE1 | 12 | 0.11 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 1 | 0.11 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 11 | 0.11 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 20 | 0.11 |
| (1,119) | 1:171:A:VAL:H | 1:114:A:ILE:O | 10 | 0.11 |
| (1,118) | 1:168:A:ILE:N | 1:122:A:VAL:O | 14 | 0.11 |
| (1,103) | 1:147:A:ASP:H | 1:175:A:PHE:O | 8 | 0.11 |
| (1,101) | 1:144:A:LEU:H | 1:99:A:HIS:O | 2 | 0.11 |
| (1,98) | 1:136:A:MET:N | 1:132:A:ARG:O | 10 | 0.11 |
| (1,97) | 1:136:A:MET:H | 1:132:A:ARG:O | 20 | 0.11 |
| (1,89) | 1:132:A:ARG:H | 1:128:A:ILE:O | 14 | 0.11 |
| (1,89) | 1:132:A:ARG:H | 1:128:A:ILE:O | 19 | 0.11 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 2 | 0.11 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 14 | 0.11 |
| (1,80) | 1:113:A:GLY:N | 1:109:A:ILE:O | 16 | 0.11 |
| (1,78) | 1:112:A:ASP:N | 1:108:A:LEU:O | 8 | 0.11 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 10 | 0.11 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 17 | 0.11 |
| (1,72) | 1:109:A:ILE:N | 1:105:A:ASN:O | 19 | 0.11 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 4 | 0.11 |
| (1,71) | 1:109:A:ILE:H | 1:105:A:ASN:O | 10 | 0.11 |
| (1,59) | 1:77:A:ASN:H | 1:64:A:ARG:O | 17 | 0.11 |
| (1,55) | 1:74:A:ILE:H | 1:32:A:ALA:O | 5 | 0.11 |
| (1,46) | 1:57:A:VAL:N | 1:53:A:LEU:O | 17 | 0.11 |
| (1,40) | 1:54:A:LYS:N | 1:50:A:MET:O | 16 | 0.11 |
| (1,39) | 1:54:A:LYS:H | 1:50:A:MET:O | 1 | 0.11 |
| (1,36) | 1:43:A:ALA:N | 1:39:A:ALA:O | 20 | 0.11 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 12 | 0.11 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 14 | 0.11 |
| (1,26) | 1:38:A:LEU:N | 1:34:A:VAL:O | 18 | 0.11 |
| (1,12) | 1:12:A:SER:N | 1:8:A:SER:O | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,8) | 1:10:A:PHE:N | 1:6:A:LYS:O | 19 | 0.11 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 18 | 0.11 |
| (1,5) | 1:9:A:LYS:H | 1:5:A:VAL:O | 2 | 0.11 |
| (1,4) | 1:8:A:SER:N | 1:4:A:MET:O | 19 | 0.11 |
| (4,442) | 1:178:A:VAL:HG22 | 1:144:A:LEU:HG | 16 | 0.1 |
| (4,425) | 1:34:A:VAL:HG21 | 1:35:A:LYS:HB2 | 17 | 0.1 |
| (4,335) | 1:146:A:VAL:HG12 | 1:158:A:PHE:HB3 | 18 | 0.1 |
| (4,290) | 1:53:A:LEU:HD23 | 1:56:A:ILE:H | 3 | 0.1 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HZ | 5 | 0.1 |
| (4,270) | 1:110:A:LEU:HG | 1:106:A:PHE:HZ | 10 | 0.1 |
| (4,235) | 1:20:A:ALA:HA | 1:20:A:ALA:H | 20 | 0.1 |
| (4,221) | 1:14:A:VAL:HG22 | 1:14:A:VAL:HA | 19 | 0.1 |
| (4,208) | 1:14:A:VAL:HG23 | 1:11:A:LEU:HA | 5 | 0.1 |
| (4,198) | 1:176:A:ILE:HD11 | 1:106:A:PHE:HE1 | 13 | 0.1 |
| (4,164) | 1:87:A:GLY:H | 1:162:A:ASN:HB3 | 19 | 0.1 |
| (4,70) | 1:130:A:THR:H | 2:201:A:NAD:H4D | 1 | 0.1 |
| (4,30) | 1:24:A:LEU:H | 1:22:A:ILE:HB | 3 | 0.1 |
| (3,20) | 1:163:A:ASN:OD1 | 2:201:A:NAD:H71N | 6 | 0.1 |
| (2,3963) | 1:123:A:HIS:HB2 | 2:201:A:NAD:H6N | 1 | 0.1 |
| (2,3924) | 1:109:A:ILE:HD11 | 2:201:A:NAD:H2A | 7 | 0.1 |
| (2,3920) | 1:115:A:LYS:H | 2:201:A:NAD:H8A | 10 | 0.1 |
| (2,3864) | 1:24:A:LEU:HA | 1:44:A:LYS:HE3 | 7 | 0.1 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 3 | 0.1 |
| (2,3838) | 1:129:A:THR:HB | 1:129:A:THR:HG22 | 19 | 0.1 |
| (2,3825) | 1:11:A:LEU:HD13 | 1:11:A:LEU:HB2 | 14 | 0.1 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB2 | 17 | 0.1 |
| (2,3779) | 1:96:A:VAL:HG11 | 1:95:A:ALA:HB3 | 19 | 0.1 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 2 | 0.1 |
| (2,3774) | 1:21:A:LEU:HD11 | 1:21:A:LEU:HB3 | 13 | 0.1 |
| (2,3772) | 1:151:A:MET:HE2 | 1:174:A:GLU:HG2 | 17 | 0.1 |
| (2,3764) | 1:160:A:LEU:HG | 1:160:A:LEU:HD13 | 10 | 0.1 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 6 | 0.1 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 14 | 0.1 |
| (2,3720) | 1:90:A:LYS:HE3 | 1:90:A:LYS:HD3 | 17 | 0.1 |
| (2,3703) | 1:110:A:LEU:HA | 1:110:A:LEU:HB3 | 18 | 0.1 |
| (2,3535) | 1:21:A:LEU:HD11 | 1:18:A:ASN:HB2 | 4 | 0.1 |
| (2,3519) | 1:48:A:ILE:HD12 | 1:53:A:LEU:HB2 | 6 | 0.1 |
| (2,3479) | 1:151:A:MET:HE2 | 1:171:A:VAL:HA | 12 | 0.1 |
| (2,3468) | 1:110:A:LEU:HD11 | 1:110:A:LEU:HA | 9 | 0.1 |
| (2,3405) | 1:56:A:ILE:HG22 | 1:57:A:VAL:H | 1 | 0.1 |
| (2,3376) | 1:95:A:ALA:HB3 | 1:96:A:VAL:H | 7 | 0.1 |
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 10 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,3376) | 1:95:A:ALA:HB2 | 1:96:A:VAL:H | 20 | 0.1 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 4 | 0.1 |
| (2,3375) | 1:48:A:ILE:HG13 | 1:48:A:ILE:H | 10 | 0.1 |
| (2,3371) | 1:20:A:ALA:HB3 | 1:18:A:ASN:HD21 | 17 | 0.1 |
| (2,3362) | 1:39:A:ALA:HB3 | 1:40:A:LYS:H | 4 | 0.1 |
| (2,3302) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 13 | 0.1 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 10 | 0.1 |
| (2,3269) | 1:34:A:VAL:HG21 | 1:34:A:VAL:H | 18 | 0.1 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 4 | 0.1 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 16 | 0.1 |
| (2,3256) | 1:160:A:LEU:HD21 | 1:160:A:LEU:HB2 | 17 | 0.1 |
| (2,3234) | 1:171:A:VAL:HA | 1:171:A:VAL:HG11 | 1 | 0.1 |
| (2,3197) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 4 | 0.1 |
| (2,3197) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 7 | 0.1 |
| (2,3197) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HB | 10 | 0.1 |
| (2,3184) | 1:92:A:VAL:HG21 | 1:92:A:VAL:H | 7 | 0.1 |
| (2,3184) | 1:92:A:VAL:HG21 | 1:92:A:VAL:H | 10 | 0.1 |
| (2,3184) | 1:92:A:VAL:HG21 | 1:92:A:VAL:H | 13 | 0.1 |
| (2,3180) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 2 | 0.1 |
| (2,3180) | 1:114:A:ILE:HD11 | 1:114:A:ILE:HG21 | 9 | 0.1 |
| (2,3173) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 2 | 0.1 |
| (2,3173) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 6 | 0.1 |
| (2,3173) | 1:176:A:ILE:HD11 | 1:176:A:ILE:HA | 20 | 0.1 |
| (2,3157) | 1:176:A:ILE:HG21 | 1:176:A:ILE:H | 14 | 0.1 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 5 | 0.1 |
| (2,2987) | 1:38:A:LEU:H | 1:37:A:LEU:H | 7 | 0.1 |
| (2,2980) | 1:40:A:LYS:H | 1:39:A:ALA:H | 5 | 0.1 |
| (2,2980) | 1:40:A:LYS:H | 1:39:A:ALA:H | 16 | 0.1 |
| (2,2949) | 1:165:A:VAL:H | 1:91:A:GLN:HE22 | 14 | 0.1 |
| (2,2822) | 1:74:A:ILE:H | 1:73:A:LYS:HB2 | 1 | 0.1 |
| (2,2822) | 1:74:A:ILE:H | 1:73:A:LYS:HB2 | 18 | 0.1 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 2 | 0.1 |
| (2,2756) | 1:59:A:THR:HG21 | 1:59:A:THR:H | 15 | 0.1 |
| (2,2748) | 1:86:A:LEU:HD11 | 1:87:A:GLY:H | 5 | 0.1 |
| (2,2680) | 1:113:A:GLY:H | 1:109:A:ILE:HG21 | 7 | 0.1 |
| (2,2664) | 1:132:A:ARG:H | 1:126:A:GLN:HE22 | 20 | 0.1 |
| (2,2657) | 1:126:A:GLN:HE21 | 1:166:A:TRP:HB2 | 8 | 0.1 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 9 | 0.1 |
| (2,2595) | 1:14:A:VAL:HG12 | 1:14:A:VAL:H | 19 | 0.1 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 4 | 0.1 |
| (2,2593) | 1:14:A:VAL:H | 1:11:A:LEU:HA | 18 | 0.1 |
| (2,2520) | 1:8:A:SER:H | 1:6:A:LYS:HA | 10 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,2520) | 1:8:A:SER:H | 1:6:A:LYS:HA | 17 | 0.1 |
| (2,2520) | 1:8:A:SER:H | 1:6:A:LYS:HA | 20 | 0.1 |
| (2,2492) | 1:129:A:THR:HG21 | 1:129:A:THR:H | 17 | 0.1 |
| (2,2360) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 17 | 0.1 |
| (2,2221) | 1:168:A:ILE:HD12 | 1:157:A:ASP:H | 20 | 0.1 |
| (2,2212) | 1:53:A:LEU:H | 1:48:A:ILE:HG12 | 1 | 0.1 |
| (2,2210) | 1:48:A:ILE:HD12 | 1:53:A:LEU:H | 5 | 0.1 |
| (2,2197) | 1:109:A:ILE:H | 1:102:A:ALA:H | 12 | 0.1 |
| (2,2169) | 1:76:A:ALA:H | 1:15:A:LEU:HB2 | 20 | 0.1 |
| (2,2142) | 1:66:A:ALA:H | 1:67:A:PHE:HB3 | 12 | 0.1 |
| (2,2132) | 1:56:A:ILE:HD11 | 1:56:A:ILE:H | 15 | 0.1 |
| (2,2078) | 1:177:A:LYS:HG2 | 1:178:A:VAL:H | 16 | 0.1 |
| (2,2077) | 1:177:A:LYS:HD2 | 1:178:A:VAL:H | 14 | 0.1 |
| (2,2052) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 9 | 0.1 |
| (2,2010) | 1:34:A:VAL:H | 1:73:A:LYS:HA | 12 | 0.1 |
| (2,1984) | 1:106:A:PHE:HD1 | 1:106:A:PHE:HE1 | 6 | 0.1 |
| (2,1984) | 1:106:A:PHE:HD1 | 1:106:A:PHE:HE1 | 10 | 0.1 |
| (2,1984) | 1:106:A:PHE:HD1 | 1:106:A:PHE:HE1 | 14 | 0.1 |
| (2,1984) | 1:106:A:PHE:HD1 | 1:106:A:PHE:HE1 | 15 | 0.1 |
| (2,1964) | 1:15:A:LEU:HD11 | 1:65:A:PHE:HD1 | 4 | 0.1 |
| (2,1879) | 1:34:A:VAL:HG21 | 1:74:A:ILE:H | 16 | 0.1 |
| (2,1866) | 1:109:A:ILE:HD13 | 1:109:A:ILE:HG12 | 2 | 0.1 |
| (2,1842) | 1:11:A:LEU:HD21 | 1:11:A:LEU:HB2 | 1 | 0.1 |
| (2,1829) | 1:22:A:ILE:HG22 | 1:44:A:LYS:HB3 | 3 | 0.1 |
| (2,1811) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 19 | 0.1 |
| (2,1805) | 1:21:A:LEU:HD22 | 1:21:A:LEU:HB3 | 13 | 0.1 |
| (2,1779) | 1:83:A:GLU:HB2 | 1:86:A:LEU:HD23 | 10 | 0.1 |
| (2,1778) | 1:57:A:VAL:HG12 | 1:57:A:VAL:HB | 14 | 0.1 |
| (2,1776) | 1:22:A:ILE:HB | 1:22:A:ILE:HG22 | 16 | 0.1 |
| (2,1745) | 1:34:A:VAL:HA | 1:37:A:LEU:HD21 | 12 | 0.1 |
| (2,1733) | 1:7:A:VAL:HA | 1:7:A:VAL:HB | 6 | 0.1 |
| (2,1733) | 1:7:A:VAL:HA | 1:7:A:VAL:HB | 7 | 0.1 |
| (2,1713) | 1:146:A:VAL:HG11 | 1:146:A:VAL:HA | 14 | 0.1 |
| (2,1687) | 1:96:A:VAL:HG21 | 1:96:A:VAL:HA | 8 | 0.1 |
| (2,1540) | 1:56:A:ILE:HG23 | 1:56:A:ILE:HA | 14 | 0.1 |
| (2,1474) | 1:110:A:LEU:HD22 | 1:110:A:LEU:H | 10 | 0.1 |
| (2,1447) | 1:146:A:VAL:HG13 | 1:146:A:VAL:H | 8 | 0.1 |
| (2,1440) | 1:37:A:LEU:HD12 | 1:37:A:LEU:H | 13 | 0.1 |
| (2,1440) | 1:37:A:LEU:HD13 | 1:37:A:LEU:H | 17 | 0.1 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 2 | 0.1 |
| (2,1433) | 1:21:A:LEU:HD11 | 1:21:A:LEU:H | 13 | 0.1 |
| (2,1432) | 1:38:A:LEU:HD12 | 1:39:A:ALA:H | 2 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,1432) | 1:38:A:LEU:HD12 | 1:39:A:ALA:H | 5 | 0.1 |
| (2,1399) | 1:86:A:LEU:HG | 1:86:A:LEU:H | 17 | 0.1 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 3 | 0.1 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 4 | 0.1 |
| (2,1328) | 1:82:A:VAL:HA | 1:83:A:GLU:H | 14 | 0.1 |
| (2,1296) | 1:57:A:VAL:HG13 | 1:65:A:PHE:HB3 | 1 | 0.1 |
| (2,1211) | 1:177:A:LYS:HD2 | 1:177:A:LYS:HA | 15 | 0.1 |
| (2,1207) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 2 | 0.1 |
| (2,1207) | 1:109:A:ILE:HG13 | 1:114:A:ILE:HD11 | 17 | 0.1 |
| (2,1110) | 1:76:A:ALA:H | 1:75:A:ARG:H | 4 | 0.1 |
| (2,1110) | 1:76:A:ALA:H | 1:75:A:ARG:H | 5 | 0.1 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 7 | 0.1 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 11 | 0.1 |
| (2,1019) | 1:52:A:GLU:H | 1:53:A:LEU:H | 14 | 0.1 |
| (2,1018) | 1:38:A:LEU:H | 1:37:A:LEU:H | 10 | 0.1 |
| (2,956) | 1:58:A:GLU:H | 1:57:A:VAL:H | 16 | 0.1 |
| (2,950) | 1:76:A:ALA:H | 1:76:A:ALA:HA | 10 | 0.1 |
| (2,950) | 1:76:A:ALA:H | 1:76:A:ALA:HA | 13 | 0.1 |
| (2,811) | 1:14:A:VAL:HG23 | 1:22:A:ILE:H | 2 | 0.1 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 16 | 0.1 |
| (2,809) | 1:22:A:ILE:H | 1:22:A:ILE:HG12 | 19 | 0.1 |
| (2,673) | 1:70:A:ASN:HD22 | 1:50:A:MET:HG3 | 16 | 0.1 |
| (2,673) | 1:70:A:ASN:HD22 | 1:50:A:MET:HG3 | 20 | 0.1 |
| (2,655) | 1:29:A:ASN:H | 1:29:A:ASN:HD22 | 2 | 0.1 |
| (2,647) | 1:14:A:VAL:H | 1:13:A:LEU:HB2 | 6 | 0.1 |
| (2,453) | 1:34:A:VAL:HB | 1:35:A:LYS:H | 3 | 0.1 |
| (2,445) | 1:36:A:GLU:H | 1:36:A:GLU:HB3 | 2 | 0.1 |
| (2,439) | 1:55:A:HIS:H | 1:54:A:LYS:HB2 | 8 | 0.1 |
| (2,431) | 1:73:A:LYS:H | 1:34:A:VAL:HG21 | 12 | 0.1 |
| (2,393) | 1:57:A:VAL:H | 1:67:A:PHE:HE1 | 14 | 0.1 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 1 | 0.1 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 4 | 0.1 |
| (2,391) | 1:28:A:ALA:H | 1:27:A:ASP:HB3 | 6 | 0.1 |
| (2,305) | 1:42:A:LYS:HA | 1:46:A:HIS:H | 5 | 0.1 |
| (2,243) | 1:53:A:LEU:H | 1:53:A:LEU:HD11 | 11 | 0.1 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 16 | 0.1 |
| (2,227) | 1:82:A:VAL:HB | 1:82:A:VAL:H | 18 | 0.1 |
| (2,197) | 1:24:A:LEU:HA | 1:24:A:LEU:H | 2 | 0.1 |
| (2,96) | 1:25:A:ASP:HB3 | 1:25:A:ASP:H | 2 | 0.1 |
| (2,62) | 1:178:A:VAL:H | 1:177:A:LYS:H | 15 | 0.1 |
| (2,42) | 1:148:A:ALA:H | 1:148:A:ALA:HB1 | 17 | 0.1 |
| (1,125) | 1:177:A:LYS:H | 1:145:A:SER:O | 7 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,119) | 1:171:A:VAL:H | 1:114:A:ILE:O | 9 | 0.1 |
| (1,90) | 1:132:A:ARG:N | 1:128:A:ILE:O | 8 | 0.1 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 5 | 0.1 |
| (1,73) | 1:110:A:LEU:H | 1:106:A:PHE:O | 13 | 0.1 |
| (1,64) | 1:99:A:HIS:N | 1:144:A:LEU:O | 3 | 0.1 |
| (1,60) | 1:77:A:ASN:N | 1:64:A:ARG:O | 20 | 0.1 |
| (1,59) | 1:77:A:ASN:H | 1:64:A:ARG:O | 12 | 0.1 |
| (1,54) | 1:66:A:ALA:N | 1:75:A:ARG:O | 8 | 0.1 |
| (1,39) | 1:54:A:LYS:H | 1:50:A:MET:O | 20 | 0.1 |
| (1,29) | 1:40:A:LYS:H | 1:36:A:GLU:O | 7 | 0.1 |
| (1,24) | 1:37:A:LEU:N | 1:33:A:PRO:O | 11 | 0.1 |
| (1,7) | 1:10:A:PHE:H | 1:6:A:LYS:O | 1 | 0.1 |

# 10 Dihedral-angle violation analysis

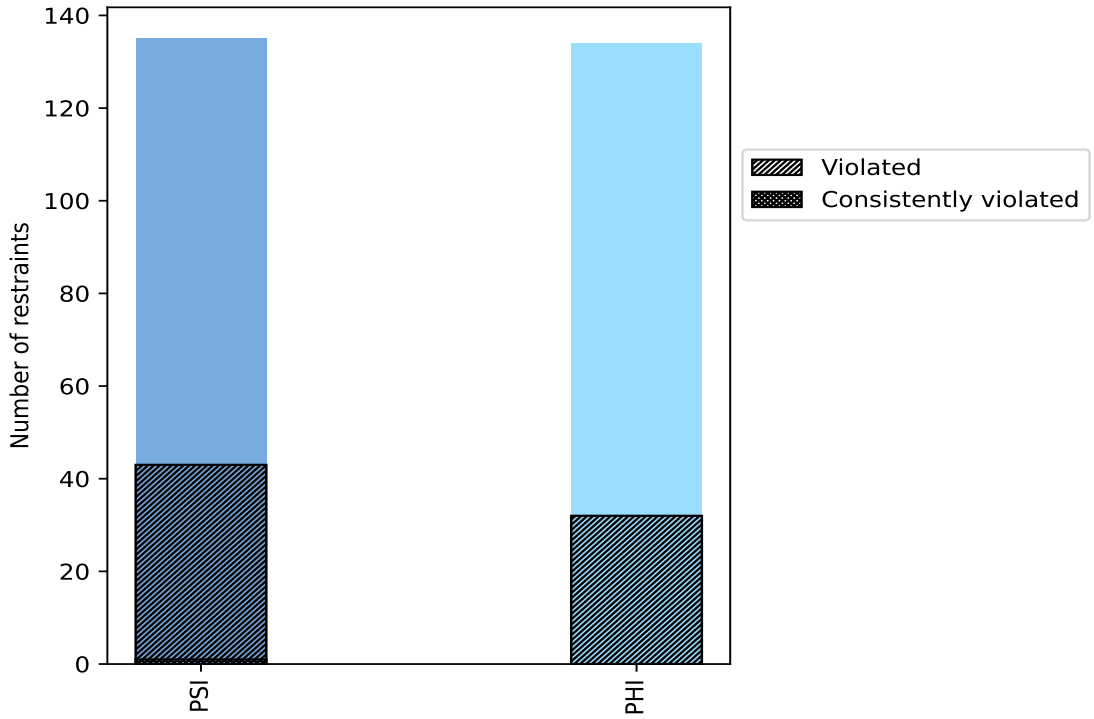
## 10.1 Summary of dihedral-angle violations

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

| Angle type | Count | %[1] | Violated[3] | | | Consistently Violated[4] | | |
|---|---|---|---|---|---|---|---|---|
| | | | Count | %[2] | %[1] | Count | %[2] | %[1] |
| PSI | 135 | 50.2 | 43 | 31.9 | 16.0 | 1 | 0.7 | 0.4 |
| PHI | 134 | 49.8 | 32 | 23.9 | 11.9 | 0 | 0.0 | 0.0 |
| Total | 269 | 100.0 | 75 | 27.9 | 27.9 | 1 | 0.4 | 0.4 |

[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



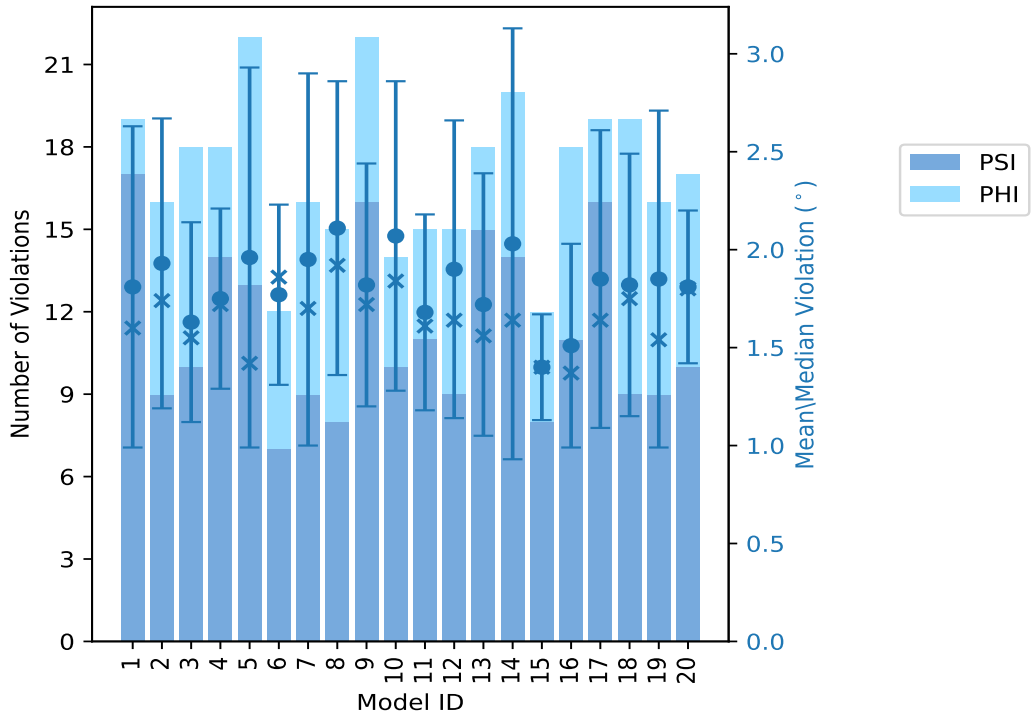

Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°) |
|---|---|---|---|---|---|---|---|
| | PSI | PHI | Total | | | | |
| 1 | 17 | 2 | 19 | 1.81 | 4.13 | 0.82 | 1.6 |
| 2 | 9 | 7 | 16 | 1.93 | 3.25 | 0.74 | 1.74 |
| 3 | 10 | 8 | 18 | 1.63 | 2.57 | 0.51 | 1.55 |
| 4 | 14 | 4 | 18 | 1.75 | 2.54 | 0.46 | 1.72 |
| 5 | 13 | 9 | 22 | 1.96 | 4.43 | 0.97 | 1.42 |
| 6 | 7 | 5 | 12 | 1.77 | 2.57 | 0.46 | 1.86 |
| 7 | 9 | 7 | 16 | 1.95 | 3.98 | 0.95 | 1.7 |
| 8 | 8 | 7 | 15 | 2.11 | 3.6 | 0.75 | 1.92 |
| 9 | 16 | 6 | 22 | 1.82 | 3.36 | 0.62 | 1.72 |
| 10 | 10 | 4 | 14 | 2.07 | 3.51 | 0.79 | 1.84 |
| 11 | 11 | 4 | 15 | 1.68 | 2.57 | 0.5 | 1.61 |
| 12 | 9 | 6 | 15 | 1.9 | 3.69 | 0.76 | 1.64 |
| 13 | 15 | 3 | 18 | 1.72 | 3.47 | 0.67 | 1.56 |
| 14 | 14 | 6 | 20 | 2.03 | 4.91 | 1.1 | 1.64 |
| 15 | 8 | 4 | 12 | 1.4 | 2.01 | 0.27 | 1.4 |
| 16 | 11 | 7 | 18 | 1.51 | 2.86 | 0.52 | 1.37 |
| 17 | 16 | 3 | 19 | 1.85 | 4.12 | 0.76 | 1.64 |
| 18 | 9 | 10 | 19 | 1.82 | 3.76 | 0.67 | 1.75 |
| 19 | 9 | 7 | 16 | 1.85 | 3.93 | 0.86 | 1.54 |
| 20 | 10 | 7 | 17 | 1.81 | 2.41 | 0.39 | 1.8 |

### 10.2.1 Bar graph : Dihedral violation statistics for each model




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

## 10.3 Dihedral-angle violation statistics for the ensemble

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

| Number of violated restraints | | | Fraction of the ensemble | |
|---|---|---|---|---|
| PSI | PHI | Total | Count[1] | % |
| 10 | 11 | 21 | 1 | 5.0 |
| 8 | 6 | 14 | 2 | 10.0 |
| 7 | 5 | 12 | 3 | 15.0 |
| 1 | 0 | 1 | 4 | 20.0 |
| 1 | 2 | 3 | 5 | 25.0 |
| 3 | 3 | 6 | 6 | 30.0 |
| 2 | 1 | 3 | 7 | 35.0 |
| 3 | 1 | 4 | 8 | 40.0 |
| 0 | 1 | 1 | 9 | 45.0 |
| 1 | 0 | 1 | 10 | 50.0 |
| 2 | 0 | 2 | 11 | 55.0 |

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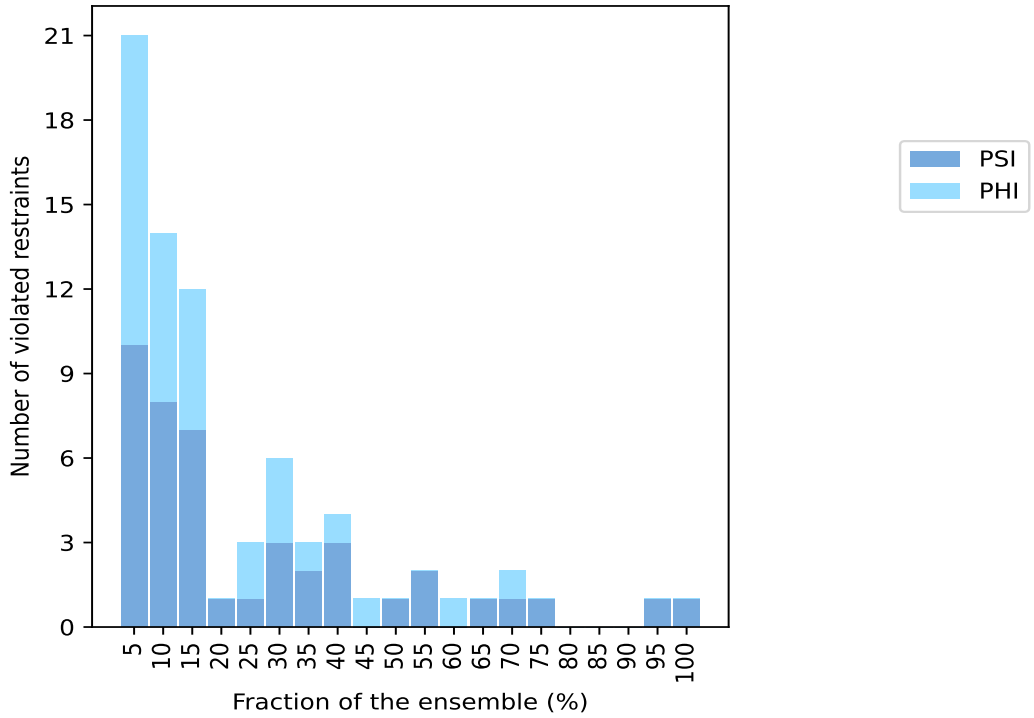
| Number of violated restraints | | | Fraction of the ensemble | |
|---|---|---|---|---|
| PSI | PHI | Total | Count[1] | % |
| 0 | 1 | 1 | 12 | 60.0 |
| 1 | 0 | 1 | 13 | 65.0 |
| 1 | 1 | 2 | 14 | 70.0 |
| 1 | 0 | 1 | 15 | 75.0 |
| 0 | 0 | 0 | 16 | 80.0 |
| 0 | 0 | 0 | 17 | 85.0 |
| 0 | 0 | 0 | 18 | 90.0 |
| 1 | 0 | 1 | 19 | 95.0 |
| 1 | 0 | 1 | 20 | 100.0 |

[1] Number of models with violations

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

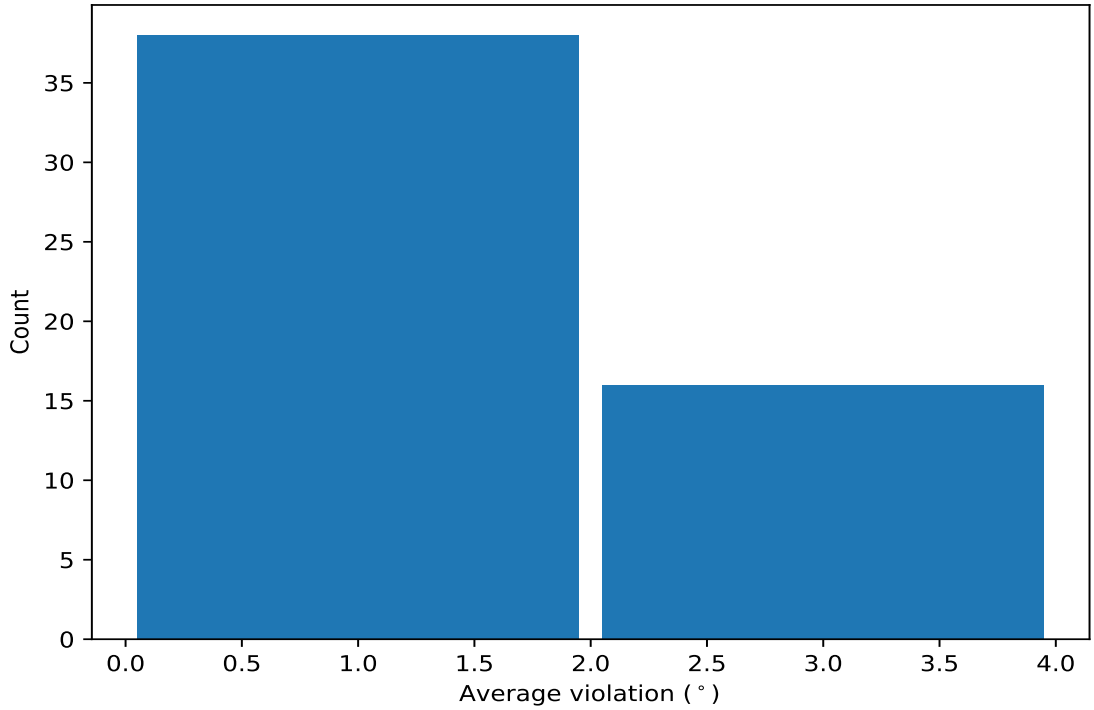



## 10.4 Most violated dihedral-angle restraints in the ensemble

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble




### 10.4.2 Table: Most violated dihedral-angle restraints

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 |
|---|---|---|---|---|---|---|---|---|
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 20 | 2.21 | 0.53 | 2.12 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 19 | 1.9 | 0.48 | 1.79 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 15 | 1.7 | 0.38 | 1.67 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 14 | 2.46 | 1.01 | 2.24 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 14 | 1.68 | 0.5 | 1.81 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 13 | 2.45 | 0.9 | 2.57 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 12 | 1.57 | 0.45 | 1.44 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 11 | 2.03 | 0.47 | 1.96 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 11 | 1.83 | 0.54 | 1.55 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 10 | 1.32 | 0.36 | 1.15 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 9 | 1.32 | 0.37 | 1.19 |
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 8 | 2.65 | 1.21 | 2.17 |
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 8 | 1.6 | 0.47 | 1.5 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 8 | 1.52 | 0.42 | 1.44 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 8 | 1.3 | 0.35 | 1.2 |
| (1,82) | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 1:48:A:ILE:N | 7 | 2.92 | 1.24 | 2.86 |
| (1,109) | 1:60:A:ASN:C | 1:61:A:SER:N | 1:61:A:SER:CA | 1:61:A:SER:C | 7 | 2.33 | 0.8 | 2.24 |
| (1,195) | 1:138:A:HIS:N | 1:138:A:HIS:CA | 1:138:A:HIS:C | 1:139:A:GLY:N | 7 | 2.19 | 0.47 | 2.08 |
| (1,158) | 1:104:A:LYS:C | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 6 | 2.42 | 0.46 | 2.46 |
| (1,138) | 1:76:A:ALA:N | 1:76:A:ALA:CA | 1:76:A:ALA:C | 1:77:A:ASN:N | 6 | 2.36 | 0.74 | 2.1 |

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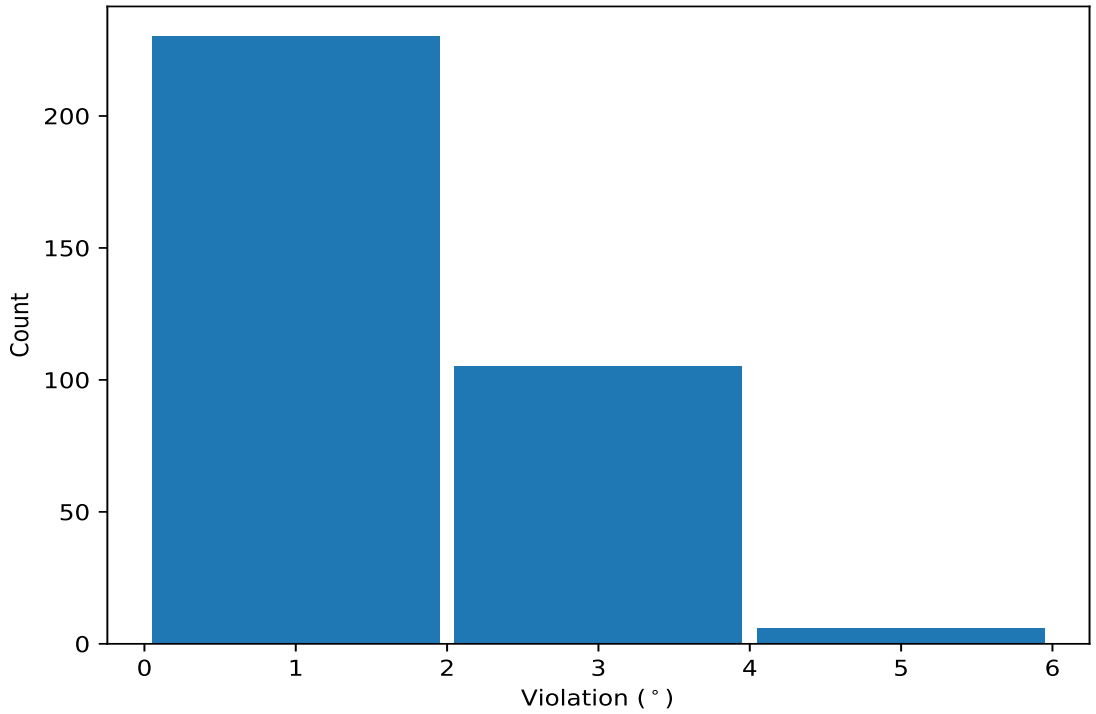
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models[1] | Mean | SD[2] | Median |
|---|---|---|---|---|---|---|---|---|
| (1,231) | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 1:161:A:SER:N | 6 | 2.28 | 0.9 | 2.21 |
| (1,154) | 1:102:A:ALA:C | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 6 | 1.62 | 0.42 | 1.65 |
| (1,58) | 1:33:A:PRO:N | 1:33:A:PRO:CA | 1:33:A:PRO:C | 1:34:A:VAL:N | 6 | 1.59 | 0.32 | 1.74 |
| (1,39) | 1:22:A:ILE:C | 1:23:A:GLY:N | 1:23:A:GLY:CA | 1:23:A:GLY:C | 6 | 1.19 | 0.09 | 1.23 |
| (1,139) | 1:76:A:ALA:C | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 5 | 2.36 | 0.79 | 2.26 |
| (1,212) | 1:150:A:GLY:C | 1:151:A:MET:N | 1:151:A:MET:CA | 1:151:A:MET:C | 5 | 1.59 | 0.28 | 1.67 |
| (1,201) | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C | 1:145:A:SER:N | 5 | 1.58 | 0.61 | 1.14 |
| (1,34) | 1:20:A:ALA:N | 1:20:A:ALA:CA | 1:20:A:ALA:C | 1:21:A:LEU:N | 4 | 1.41 | 0.14 | 1.36 |
| (1,83) | 1:47:A:GLY:C | 1:48:A:ILE:N | 1:48:A:ILE:CA | 1:48:A:ILE:C | 3 | 2.42 | 0.42 | 2.42 |
| (1,50) | 1:29:A:ASN:N | 1:29:A:ASN:CA | 1:29:A:ASN:C | 1:30:A:GLY:N | 3 | 2.38 | 0.26 | 2.48 |
| (1,207) | 1:148:A:ALA:N | 1:148:A:ALA:CA | 1:148:A:ALA:C | 1:149:A:LYS:N | 3 | 2.27 | 1.53 | 1.21 |
| (1,206) | 1:147:A:ASP:C | 1:148:A:ALA:N | 1:148:A:ALA:CA | 1:148:A:ALA:C | 3 | 1.61 | 0.18 | 1.65 |
| (1,173) | 1:112:A:ASP:N | 1:112:A:ASP:CA | 1:112:A:ASP:C | 1:113:A:GLY:N | 3 | 1.6 | 0.25 | 1.61 |
| (1,81) | 1:46:A:HIS:C | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 3 | 1.54 | 0.19 | 1.41 |
| (1,80) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C | 1:45:A:GLY:N | 3 | 1.46 | 0.4 | 1.24 |
| (1,18) | 1:12:A:SER:N | 1:12:A:SER:CA | 1:12:A:SER:C | 1:13:A:LEU:N | 3 | 1.38 | 0.28 | 1.44 |
| (1,230) | 1:159:A:TYR:C | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 3 | 1.32 | 0.32 | 1.1 |
| (1,41) | 1:23:A:GLY:C | 1:24:A:LEU:N | 1:24:A:LEU:CA | 1:24:A:LEU:C | 3 | 1.29 | 0.25 | 1.14 |
| (1,191) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C | 1:137:A:ARG:N | 3 | 1.2 | 0.04 | 1.19 |
| (1,22) | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C | 1:15:A:LEU:N | 3 | 1.15 | 0.09 | 1.2 |
| (1,107) | 1:59:A:THR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 2 | 2.68 | 0.42 | 2.68 |
| (1,112) | 1:62:A:LYS:N | 1:62:A:LYS:CA | 1:62:A:LYS:C | 1:63:A:LYS:N | 2 | 1.73 | 0.72 | 1.73 |
| (1,223) | 1:156:A:PHE:N | 1:156:A:PHE:CA | 1:156:A:PHE:C | 1:157:A:ASP:N | 2 | 1.57 | 0.05 | 1.57 |
| (1,226) | 1:157:A:ASP:C | 1:158:A:PHE:N | 1:158:A:PHE:CA | 1:158:A:PHE:C | 2 | 1.56 | 0.03 | 1.56 |
| (1,147) | 1:94:A:PRO:N | 1:94:A:PRO:CA | 1:94:A:PRO:C | 1:95:A:ALA:N | 2 | 1.56 | 0.07 | 1.56 |
| (1,36) | 1:21:A:LEU:N | 1:21:A:LEU:CA | 1:21:A:LEU:C | 1:22:A:ILE:N | 2 | 1.4 | 0.17 | 1.4 |
| (1,145) | 1:93:A:PRO:N | 1:93:A:PRO:CA | 1:93:A:PRO:C | 1:94:A:PRO:N | 2 | 1.35 | 0.0 | 1.35 |
| (1,79) | 1:43:A:ALA:C | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C | 2 | 1.31 | 0.05 | 1.31 |
| (1,266) | 1:94:A:PRO:C | 1:95:A:ALA:N | 1:95:A:ALA:CA | 1:95:A:ALA:C | 2 | 1.3 | 0.0 | 1.3 |
| (1,221) | 1:155:A:GLY:N | 1:155:A:GLY:CA | 1:155:A:GLY:C | 1:156:A:PHE:N | 2 | 1.27 | 0.06 | 1.27 |
| (1,105) | 1:58:A:GLU:C | 1:59:A:THR:N | 1:59:A:THR:CA | 1:59:A:THR:C | 2 | 1.14 | 0.1 | 1.14 |
| (1,159) | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 1:106:A:PHE:N | 2 | 1.09 | 0.01 | 1.09 |
| (1,228) | 1:158:A:PHE:C | 1:159:A:TYR:N | 1:159:A:TYR:CA | 1:159:A:TYR:C | 2 | 1.04 | 0.01 | 1.04 |
| (1,4) | 1:5:A:VAL:N | 1:5:A:VAL:CA | 1:5:A:VAL:C | 1:6:A:LYS:N | 2 | 1.02 | 0.01 | 1.02 |

[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

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 (°) |
|---|---|---|---|---|---|---|
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 14 | 4.91 |
| (1,82) | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 1:48:A:ILE:N | 14 | 4.63 |
| (1,207) | 1:148:A:ALA:N | 1:148:A:ALA:CA | 1:148:A:ALA:C | 1:149:A:LYS:N | 5 | 4.43 |
| (1,82) | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 1:48:A:ILE:N | 5 | 4.26 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 1 | 4.13 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 17 | 4.12 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 7 | 3.98 |
| (1,109) | 1:60:A:ASN:C | 1:61:A:SER:N | 1:61:A:SER:CA | 1:61:A:SER:C | 19 | 3.93 |
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 1 | 3.85 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 7 | 3.81 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 18 | 3.76 |
| (1,82) | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 1:48:A:ILE:N | 12 | 3.69 |
| (1,138) | 1:76:A:ALA:N | 1:76:A:ALA:CA | 1:76:A:ALA:C | 1:77:A:ASN:N | 8 | 3.6 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 10 | 3.51 |
| (1,231) | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 1:161:A:SER:N | 13 | 3.47 |
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 10 | 3.47 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 9 | 3.36 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 7 | 3.36 |
| (1,139) | 1:76:A:ALA:C | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 8 | 3.28 |
| (1,139) | 1:76:A:ALA:C | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 2 | 3.25 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 19 | 3.18 |

*Continued on next page...*

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,195) | 1:138:A:HIS:N | 1:138:A:HIS:CA | 1:138:A:HIS:C | 1:139:A:GLY:N | 5 | 3.18 |
| (1,231) | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 1:161:A:SER:N | 9 | 3.15 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 19 | 3.11 |
| (1,138) | 1:76:A:ALA:N | 1:76:A:ALA:CA | 1:76:A:ALA:C | 1:77:A:ASN:N | 2 | 3.09 |
| (1,107) | 1:59:A:THR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 10 | 3.09 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 12 | 3.07 |
| (1,240) | 1:164:A:GLY:C | 1:165:A:VAL:N | 1:165:A:VAL:CA | 1:165:A:VAL:C | 5 | 3.01 |
| (1,158) | 1:104:A:LYS:C | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 2 | 3.01 |
| (1,83) | 1:47:A:GLY:C | 1:48:A:ILE:N | 1:48:A:ILE:CA | 1:48:A:ILE:C | 14 | 2.93 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 8 | 2.91 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 12 | 2.9 |
| (1,82) | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 1:48:A:ILE:N | 16 | 2.86 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 14 | 2.84 |
| (1,231) | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 1:161:A:SER:N | 2 | 2.82 |
| (1,158) | 1:104:A:LYS:C | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 16 | 2.8 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 14 | 2.79 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 17 | 2.76 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 17 | 2.72 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 5 | 2.7 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 8 | 2.67 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 19 | 2.65 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 18 | 2.64 |
| (1,50) | 1:29:A:ASN:N | 1:29:A:ASN:CA | 1:29:A:ASN:C | 1:30:A:GLY:N | 10 | 2.64 |
| (1,109) | 1:60:A:ASN:C | 1:61:A:SER:N | 1:61:A:SER:CA | 1:61:A:SER:C | 7 | 2.63 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 17 | 2.59 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 8 | 2.57 |
| (1,158) | 1:104:A:LYS:C | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 11 | 2.57 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 3 | 2.57 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 6 | 2.57 |
| (1,201) | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C | 1:145:A:SER:N | 8 | 2.55 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 4 | 2.54 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 13 | 2.54 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 2 | 2.52 |
| (1,50) | 1:29:A:ASN:N | 1:29:A:ASN:CA | 1:29:A:ASN:C | 1:30:A:GLY:N | 9 | 2.48 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 11 | 2.48 |
| (1,112) | 1:62:A:LYS:N | 1:62:A:LYS:CA | 1:62:A:LYS:C | 1:63:A:LYS:N | 18 | 2.45 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 4 | 2.45 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 4 | 2.42 |
| (1,83) | 1:47:A:GLY:C | 1:48:A:ILE:N | 1:48:A:ILE:CA | 1:48:A:ILE:C | 5 | 2.42 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 1 | 2.41 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 20 | 2.41 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 20 | 2.41 |
| (1,195) | 1:138:A:HIS:N | 1:138:A:HIS:CA | 1:138:A:HIS:C | 1:139:A:GLY:N | 6 | 2.4 |
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 11 | 2.37 |
| (1,154) | 1:102:A:ALA:C | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 3 | 2.37 |
| (1,109) | 1:60:A:ASN:C | 1:61:A:SER:N | 1:61:A:SER:CA | 1:61:A:SER:C | 17 | 2.37 |
| (1,158) | 1:104:A:LYS:C | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 3 | 2.35 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 14 | 2.35 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 5 | 2.33 |
| (1,144) | 1:92:A:VAL:C | 1:93:A:PRO:N | 1:93:A:PRO:CA | 1:93:A:PRO:C | 9 | 2.32 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 14 | 2.32 |

*Continued on next page...*

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 9 | 2.3 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 10 | 2.29 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 3 | 2.27 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 20 | 2.27 |
| (1,139) | 1:76:A:ALA:C | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 18 | 2.26 |
| (1,107) | 1:59:A:THR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 18 | 2.26 |
| (1,109) | 1:60:A:ASN:C | 1:61:A:SER:N | 1:61:A:SER:CA | 1:61:A:SER:C | 9 | 2.24 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 13 | 2.22 |
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 13 | 2.22 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 4 | 2.21 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 11 | 2.2 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 12 | 2.2 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 20 | 2.18 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 3 | 2.17 |
| (1,158) | 1:104:A:LYS:C | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 18 | 2.15 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 20 | 2.15 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 13 | 2.15 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 13 | 2.14 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 10 | 2.14 |
| (1,195) | 1:138:A:HIS:N | 1:138:A:HIS:CA | 1:138:A:HIS:C | 1:139:A:GLY:N | 13 | 2.13 |
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 9 | 2.13 |
| (1,109) | 1:60:A:ASN:C | 1:61:A:SER:N | 1:61:A:SER:CA | 1:61:A:SER:C | 12 | 2.12 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 8 | 2.12 |
| (1,138) | 1:76:A:ALA:N | 1:76:A:ALA:CA | 1:76:A:ALA:C | 1:77:A:ASN:N | 18 | 2.11 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 6 | 2.11 |
| (1,138) | 1:76:A:ALA:N | 1:76:A:ALA:CA | 1:76:A:ALA:C | 1:77:A:ASN:N | 13 | 2.1 |
| (1,195) | 1:138:A:HIS:N | 1:138:A:HIS:CA | 1:138:A:HIS:C | 1:139:A:GLY:N | 4 | 2.08 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 19 | 2.08 |
| (1,82) | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 1:48:A:ILE:N | 17 | 2.07 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 12 | 2.06 |
| (1,195) | 1:138:A:HIS:N | 1:138:A:HIS:CA | 1:138:A:HIS:C | 1:139:A:GLY:N | 2 | 2.06 |
| (1,201) | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C | 1:145:A:SER:N | 20 | 2.05 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 1 | 2.03 |
| (1,50) | 1:29:A:ASN:N | 1:29:A:ASN:CA | 1:29:A:ASN:C | 1:30:A:GLY:N | 18 | 2.03 |
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 5 | 2.02 |
| (1,109) | 1:60:A:ASN:C | 1:61:A:SER:N | 1:61:A:SER:CA | 1:61:A:SER:C | 6 | 2.02 |
| (1,80) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C | 1:45:A:GLY:N | 20 | 2.02 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 15 | 2.01 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 4 | 2.0 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 6 | 1.96 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 10 | 1.95 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 17 | 1.94 |
| (1,232) | 1:160:A:LEU:C | 1:161:A:SER:N | 1:161:A:SER:CA | 1:161:A:SER:C | 7 | 1.92 |
| (1,212) | 1:150:A:GLY:C | 1:151:A:MET:N | 1:151:A:MET:CA | 1:151:A:MET:C | 3 | 1.92 |
| (1,58) | 1:33:A:PRO:N | 1:33:A:PRO:CA | 1:33:A:PRO:C | 1:34:A:VAL:N | 8 | 1.92 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 16 | 1.92 |
| (1,195) | 1:138:A:HIS:N | 1:138:A:HIS:CA | 1:138:A:HIS:C | 1:139:A:GLY:N | 1 | 1.91 |
| (1,173) | 1:112:A:ASP:N | 1:112:A:ASP:CA | 1:112:A:ASP:C | 1:113:A:GLY:N | 9 | 1.91 |
| (1,83) | 1:47:A:GLY:C | 1:48:A:ILE:N | 1:48:A:ILE:CA | 1:48:A:ILE:C | 12 | 1.91 |
| (1,82) | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 1:48:A:ILE:N | 20 | 1.91 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 11 | 1.91 |

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*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 14 | 1.9 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 4 | 1.9 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 9 | 1.9 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 6 | 1.89 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 18 | 1.89 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 2 | 1.89 |
| (1,229) | 1:159:A:TYR:N | 1:159:A:TYR:CA | 1:159:A:TYR:C | 1:160:A:LEU:N | 14 | 1.88 |
| (1,58) | 1:33:A:PRO:N | 1:33:A:PRO:CA | 1:33:A:PRO:C | 1:34:A:VAL:N | 4 | 1.84 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 7 | 1.84 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 1 | 1.83 |
| (1,212) | 1:150:A:GLY:C | 1:151:A:MET:N | 1:151:A:MET:CA | 1:151:A:MET:C | 4 | 1.82 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 6 | 1.82 |
| (1,206) | 1:147:A:ASP:C | 1:148:A:ALA:N | 1:148:A:ALA:CA | 1:148:A:ALA:C | 7 | 1.8 |
| (1,81) | 1:46:A:HIS:C | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 20 | 1.8 |
| (1,58) | 1:33:A:PRO:N | 1:33:A:PRO:CA | 1:33:A:PRO:C | 1:34:A:VAL:N | 3 | 1.8 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 5 | 1.79 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 2 | 1.79 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 16 | 1.79 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 1 | 1.79 |
| (1,230) | 1:159:A:TYR:C | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 8 | 1.77 |
| (1,154) | 1:102:A:ALA:C | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 19 | 1.77 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 18 | 1.75 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 14 | 1.74 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 9 | 1.74 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 10 | 1.74 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 7 | 1.73 |
| (1,154) | 1:102:A:ALA:C | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 11 | 1.73 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 9 | 1.73 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 17 | 1.71 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 9 | 1.71 |
| (1,219) | 1:154:A:GLY:N | 1:154:A:GLY:CA | 1:154:A:GLY:C | 1:155:A:GLY:N | 17 | 1.7 |
| (1,58) | 1:33:A:PRO:N | 1:33:A:PRO:CA | 1:33:A:PRO:C | 1:34:A:VAL:N | 2 | 1.69 |
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 7 | 1.68 |
| (1,18) | 1:12:A:SER:N | 1:12:A:SER:CA | 1:12:A:SER:C | 1:13:A:LEU:N | 11 | 1.68 |
| (1,212) | 1:150:A:GLY:C | 1:151:A:MET:N | 1:151:A:MET:CA | 1:151:A:MET:C | 19 | 1.67 |
| (1,138) | 1:76:A:ALA:N | 1:76:A:ALA:CA | 1:76:A:ALA:C | 1:77:A:ASN:N | 1 | 1.67 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 3 | 1.67 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 7 | 1.66 |
| (1,206) | 1:147:A:ASP:C | 1:148:A:ALA:N | 1:148:A:ALA:CA | 1:148:A:ALA:C | 8 | 1.65 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 12 | 1.64 |
| (1,41) | 1:23:A:GLY:C | 1:24:A:LEU:N | 1:24:A:LEU:CA | 1:24:A:LEU:C | 20 | 1.64 |
| (1,34) | 1:20:A:ALA:N | 1:20:A:ALA:CA | 1:20:A:ALA:C | 1:21:A:LEU:N | 15 | 1.64 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 17 | 1.64 |
| (1,147) | 1:94:A:PRO:N | 1:94:A:PRO:CA | 1:94:A:PRO:C | 1:95:A:ALA:N | 4 | 1.63 |
| (1,136) | 1:75:A:ARG:N | 1:75:A:ARG:CA | 1:75:A:ARG:C | 1:76:A:ALA:N | 20 | 1.63 |
| (1,223) | 1:156:A:PHE:N | 1:156:A:PHE:CA | 1:156:A:PHE:C | 1:157:A:ASP:N | 17 | 1.62 |
| (1,173) | 1:112:A:ASP:N | 1:112:A:ASP:CA | 1:112:A:ASP:C | 1:113:A:GLY:N | 1 | 1.61 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 11 | 1.61 |
| (1,158) | 1:104:A:LYS:C | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 19 | 1.61 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 11 | 1.61 |
| (1,231) | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 1:161:A:SER:N | 20 | 1.6 |

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*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,139) | 1:76:A:ALA:C | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 13 | 1.6 |
| (1,138) | 1:76:A:ALA:N | 1:76:A:ALA:CA | 1:76:A:ALA:C | 1:77:A:ASN:N | 9 | 1.6 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 1 | 1.6 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 4 | 1.59 |
| (1,226) | 1:157:A:ASP:C | 1:158:A:PHE:N | 1:158:A:PHE:CA | 1:158:A:PHE:C | 18 | 1.58 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 9 | 1.58 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 4 | 1.58 |
| (1,195) | 1:138:A:HIS:N | 1:138:A:HIS:CA | 1:138:A:HIS:C | 1:139:A:GLY:N | 15 | 1.57 |
| (1,154) | 1:102:A:ALA:C | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 16 | 1.57 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 1 | 1.57 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 3 | 1.57 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 5 | 1.56 |
| (1,36) | 1:21:A:LEU:N | 1:21:A:LEU:CA | 1:21:A:LEU:C | 1:22:A:ILE:N | 1 | 1.56 |
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 15 | 1.55 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 10 | 1.55 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 14 | 1.55 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 8 | 1.55 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 1 | 1.54 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 12 | 1.54 |
| (1,226) | 1:157:A:ASP:C | 1:158:A:PHE:N | 1:158:A:PHE:CA | 1:158:A:PHE:C | 20 | 1.53 |
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 3 | 1.53 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 13 | 1.53 |
| (1,223) | 1:156:A:PHE:N | 1:156:A:PHE:CA | 1:156:A:PHE:C | 1:157:A:ASP:N | 4 | 1.52 |
| (1,231) | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 1:161:A:SER:N | 10 | 1.51 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 18 | 1.51 |
| (1,146) | 1:93:A:PRO:C | 1:94:A:PRO:N | 1:94:A:PRO:CA | 1:94:A:PRO:C | 6 | 1.51 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 8 | 1.51 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 6 | 1.5 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 15 | 1.5 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 17 | 1.49 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 19 | 1.48 |
| (1,147) | 1:94:A:PRO:N | 1:94:A:PRO:CA | 1:94:A:PRO:C | 1:95:A:ALA:N | 14 | 1.48 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 17 | 1.46 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 4 | 1.45 |
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 2 | 1.44 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 18 | 1.44 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 5 | 1.44 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 2 | 1.44 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 14 | 1.44 |
| (1,18) | 1:12:A:SER:N | 1:12:A:SER:CA | 1:12:A:SER:C | 1:13:A:LEU:N | 16 | 1.44 |
| (1,139) | 1:76:A:ALA:C | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 9 | 1.43 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 5 | 1.41 |
| (1,81) | 1:46:A:HIS:C | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 16 | 1.41 |
| (1,25) | 1:15:A:LEU:C | 1:16:A:ARG:N | 1:16:A:ARG:CA | 1:16:A:ARG:C | 5 | 1.41 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 15 | 1.4 |
| (1,177) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C | 1:130:A:THR:N | 5 | 1.4 |
| (1,157) | 1:104:A:LYS:N | 1:104:A:LYS:CA | 1:104:A:LYS:C | 1:105:A:ASN:N | 15 | 1.4 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 9 | 1.4 |
| (1,81) | 1:46:A:HIS:C | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 5 | 1.4 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 16 | 1.39 |
| (1,34) | 1:20:A:ALA:N | 1:20:A:ALA:CA | 1:20:A:ALA:C | 1:21:A:LEU:N | 17 | 1.39 |

*Continued on next page...*

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 12 | 1.38 |
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 16 | 1.37 |
| (1,206) | 1:147:A:ASP:C | 1:148:A:ALA:N | 1:148:A:ALA:CA | 1:148:A:ALA:C | 14 | 1.37 |
| (1,244) | 1:166:A:TRP:C | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C | 18 | 1.36 |
| (1,108) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1:61:A:SER:N | 16 | 1.36 |
| (1,79) | 1:43:A:ALA:C | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C | 5 | 1.36 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 12 | 1.36 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 15 | 1.36 |
| (1,145) | 1:93:A:PRO:N | 1:93:A:PRO:CA | 1:93:A:PRO:C | 1:94:A:PRO:N | 5 | 1.35 |
| (1,145) | 1:93:A:PRO:N | 1:93:A:PRO:CA | 1:93:A:PRO:C | 1:94:A:PRO:N | 20 | 1.35 |
| (1,74) | 1:41:A:MET:N | 1:41:A:MET:CA | 1:41:A:MET:C | 1:42:A:LYS:N | 16 | 1.35 |
| (1,251) | 1:170:A:PHE:N | 1:170:A:PHE:CA | 1:170:A:PHE:C | 1:171:A:VAL:N | 5 | 1.33 |
| (1,221) | 1:155:A:GLY:N | 1:155:A:GLY:CA | 1:155:A:GLY:C | 1:156:A:PHE:N | 9 | 1.33 |
| (1,34) | 1:20:A:ALA:N | 1:20:A:ALA:CA | 1:20:A:ALA:C | 1:21:A:LEU:N | 10 | 1.33 |
| (1,241) | 1:165:A:VAL:N | 1:165:A:VAL:CA | 1:165:A:VAL:C | 1:166:A:TRP:N | 11 | 1.32 |
| (1,266) | 1:94:A:PRO:C | 1:95:A:ALA:N | 1:95:A:ALA:CA | 1:95:A:ALA:C | 4 | 1.3 |
| (1,266) | 1:94:A:PRO:C | 1:95:A:ALA:N | 1:95:A:ALA:CA | 1:95:A:ALA:C | 13 | 1.3 |
| (1,212) | 1:150:A:GLY:C | 1:151:A:MET:N | 1:151:A:MET:CA | 1:151:A:MET:C | 20 | 1.3 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 1 | 1.29 |
| (1,173) | 1:112:A:ASP:N | 1:112:A:ASP:CA | 1:112:A:ASP:C | 1:113:A:GLY:N | 19 | 1.29 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 10 | 1.29 |
| (1,34) | 1:20:A:ALA:N | 1:20:A:ALA:CA | 1:20:A:ALA:C | 1:21:A:LEU:N | 9 | 1.29 |
| (1,39) | 1:22:A:ILE:C | 1:23:A:GLY:N | 1:23:A:GLY:CA | 1:23:A:GLY:C | 16 | 1.28 |
| (1,38) | 1:22:A:ILE:N | 1:22:A:ILE:CA | 1:22:A:ILE:C | 1:23:A:GLY:N | 2 | 1.28 |
| (1,39) | 1:22:A:ILE:C | 1:23:A:GLY:N | 1:23:A:GLY:CA | 1:23:A:GLY:C | 2 | 1.27 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 20 | 1.26 |
| (1,79) | 1:43:A:ALA:C | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C | 20 | 1.26 |
| (1,191) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C | 1:137:A:ARG:N | 14 | 1.25 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 19 | 1.24 |
| (1,105) | 1:58:A:GLU:C | 1:59:A:THR:N | 1:59:A:THR:CA | 1:59:A:THR:C | 8 | 1.24 |
| (1,80) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C | 1:45:A:GLY:N | 17 | 1.24 |
| (1,39) | 1:22:A:ILE:C | 1:23:A:GLY:N | 1:23:A:GLY:CA | 1:23:A:GLY:C | 10 | 1.23 |
| (1,36) | 1:21:A:LEU:N | 1:21:A:LEU:CA | 1:21:A:LEU:C | 1:22:A:ILE:N | 3 | 1.23 |
| (1,22) | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C | 1:15:A:LEU:N | 11 | 1.23 |
| (1,212) | 1:150:A:GLY:C | 1:151:A:MET:N | 1:151:A:MET:CA | 1:151:A:MET:C | 12 | 1.22 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 13 | 1.22 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 1 | 1.22 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 1 | 1.22 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 11 | 1.22 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 16 | 1.22 |
| (1,39) | 1:22:A:ILE:C | 1:23:A:GLY:N | 1:23:A:GLY:CA | 1:23:A:GLY:C | 6 | 1.22 |
| (1,221) | 1:155:A:GLY:N | 1:155:A:GLY:CA | 1:155:A:GLY:C | 1:156:A:PHE:N | 16 | 1.21 |
| (1,207) | 1:148:A:ALA:N | 1:148:A:ALA:CA | 1:148:A:ALA:C | 1:149:A:LYS:N | 9 | 1.21 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 3 | 1.21 |
| (1,58) | 1:33:A:PRO:N | 1:33:A:PRO:CA | 1:33:A:PRO:C | 1:34:A:VAL:N | 12 | 1.21 |
| (1,154) | 1:102:A:ALA:C | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 18 | 1.2 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 19 | 1.2 |
| (1,22) | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C | 1:15:A:LEU:N | 7 | 1.2 |
| (1,243) | 1:166:A:TRP:N | 1:166:A:TRP:CA | 1:166:A:TRP:C | 1:167:A:LEU:N | 17 | 1.19 |
| (1,222) | 1:155:A:GLY:C | 1:156:A:PHE:N | 1:156:A:PHE:CA | 1:156:A:PHE:C | 4 | 1.19 |
| (1,191) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C | 1:137:A:ARG:N | 7 | 1.19 |

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*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 8 | 1.19 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 3 | 1.19 |
| (1,114) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1:64:A:ARG:N | 19 | 1.19 |
| (1,19) | 1:12:A:SER:C | 1:13:A:LEU:N | 1:13:A:LEU:CA | 1:13:A:LEU:C | 7 | 1.19 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 13 | 1.18 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 10 | 1.18 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 15 | 1.18 |
| (1,207) | 1:148:A:ALA:N | 1:148:A:ALA:CA | 1:148:A:ALA:C | 1:149:A:LYS:N | 11 | 1.17 |
| (1,235) | 1:162:A:ASN:N | 1:162:A:ASN:CA | 1:162:A:ASN:C | 1:163:A:ASN:N | 6 | 1.16 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 5 | 1.16 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 17 | 1.16 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 2 | 1.16 |
| (1,191) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C | 1:137:A:ARG:N | 13 | 1.15 |
| (1,201) | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C | 1:145:A:SER:N | 1 | 1.14 |
| (1,41) | 1:23:A:GLY:C | 1:24:A:LEU:N | 1:24:A:LEU:CA | 1:24:A:LEU:C | 3 | 1.14 |
| (1,201) | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C | 1:145:A:SER:N | 3 | 1.13 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 8 | 1.13 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 19 | 1.13 |
| (1,205) | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 1:148:A:ALA:N | 9 | 1.12 |
| (1,231) | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 1:161:A:SER:N | 19 | 1.11 |
| (1,80) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C | 1:45:A:GLY:N | 14 | 1.11 |
| (1,230) | 1:159:A:TYR:C | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 6 | 1.1 |
| (1,204) | 1:146:A:VAL:C | 1:147:A:ASP:N | 1:147:A:ASP:CA | 1:147:A:ASP:C | 12 | 1.1 |
| (1,202) | 1:144:A:LEU:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 7 | 1.1 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 2 | 1.1 |
| (1,159) | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 1:106:A:PHE:N | 18 | 1.1 |
| (1,41) | 1:23:A:GLY:C | 1:24:A:LEU:N | 1:24:A:LEU:CA | 1:24:A:LEU:C | 5 | 1.1 |
| (1,230) | 1:159:A:TYR:C | 1:160:A:LEU:N | 1:160:A:LEU:CA | 1:160:A:LEU:C | 18 | 1.09 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 11 | 1.09 |
| (1,140) | 1:77:A:ASN:N | 1:77:A:ASN:CA | 1:77:A:ASN:C | 1:78:A:GLN:N | 12 | 1.09 |
| (1,58) | 1:33:A:PRO:N | 1:33:A:PRO:CA | 1:33:A:PRO:C | 1:34:A:VAL:N | 5 | 1.09 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 9 | 1.09 |
| (1,39) | 1:22:A:ILE:C | 1:23:A:GLY:N | 1:23:A:GLY:CA | 1:23:A:GLY:C | 15 | 1.09 |
| (1,159) | 1:105:A:ASN:N | 1:105:A:ASN:CA | 1:105:A:ASN:C | 1:106:A:PHE:N | 11 | 1.08 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 3 | 1.08 |
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 5 | 1.07 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 3 | 1.07 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 14 | 1.07 |
| (1,168) | 1:109:A:ILE:C | 1:110:A:LEU:N | 1:110:A:LEU:CA | 1:110:A:LEU:C | 16 | 1.07 |
| (1,154) | 1:102:A:ALA:C | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 2 | 1.07 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 1 | 1.07 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 7 | 1.07 |
| (1,43) | 1:24:A:LEU:C | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C | 15 | 1.06 |
| (1,28) | 1:17:A:HIS:N | 1:17:A:HIS:CA | 1:17:A:HIS:C | 1:18:A:ASN:N | 16 | 1.06 |
| (1,228) | 1:158:A:PHE:C | 1:159:A:TYR:N | 1:159:A:TYR:CA | 1:159:A:TYR:C | 18 | 1.05 |
| (1,201) | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C | 1:145:A:SER:N | 15 | 1.05 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 7 | 1.05 |
| (1,228) | 1:158:A:PHE:C | 1:159:A:TYR:N | 1:159:A:TYR:CA | 1:159:A:TYR:C | 14 | 1.04 |
| (1,141) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C | 1:92:A:VAL:N | 16 | 1.04 |
| (1,105) | 1:58:A:GLU:C | 1:59:A:THR:N | 1:59:A:THR:CA | 1:59:A:THR:C | 3 | 1.04 |
| (1,86) | 1:49:A:SER:N | 1:49:A:SER:CA | 1:49:A:SER:C | 1:50:A:MET:N | 17 | 1.04 |

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*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,264) | 1:176:A:ILE:C | 1:177:A:LYS:N | 1:177:A:LYS:CA | 1:177:A:LYS:C | 18 | 1.03 |
| (1,109) | 1:60:A:ASN:C | 1:61:A:SER:N | 1:61:A:SER:CA | 1:61:A:SER:C | 14 | 1.03 |
| (1,39) | 1:22:A:ILE:C | 1:23:A:GLY:N | 1:23:A:GLY:CA | 1:23:A:GLY:C | 14 | 1.03 |
| (1,4) | 1:5:A:VAL:N | 1:5:A:VAL:CA | 1:5:A:VAL:C | 1:6:A:LYS:N | 4 | 1.03 |
| (1,220) | 1:154:A:GLY:C | 1:155:A:GLY:N | 1:155:A:GLY:CA | 1:155:A:GLY:C | 17 | 1.02 |
| (1,102) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLU:N | 13 | 1.02 |
| (1,90) | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1:52:A:GLU:N | 13 | 1.02 |
| (1,22) | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C | 1:15:A:LEU:N | 19 | 1.02 |
| (1,4) | 1:5:A:VAL:N | 1:5:A:VAL:CA | 1:5:A:VAL:C | 1:6:A:LYS:N | 16 | 1.02 |
| (1,236) | 1:162:A:ASN:C | 1:163:A:ASN:N | 1:163:A:ASN:CA | 1:163:A:ASN:C | 9 | 1.01 |
| (1,112) | 1:62:A:LYS:N | 1:62:A:LYS:CA | 1:62:A:LYS:C | 1:63:A:LYS:N | 13 | 1.01 |
| (1,82) | 1:47:A:GLY:N | 1:47:A:GLY:CA | 1:47:A:GLY:C | 1:48:A:ILE:N | 1 | 1.01 |
| (1,18) | 1:12:A:SER:N | 1:12:A:SER:CA | 1:12:A:SER:C | 1:13:A:LEU:N | 4 | 1.01 |
| (1,124) | 1:69:A:GLU:N | 1:69:A:GLU:CA | 1:69:A:GLU:C | 1:70:A:ASN:N | 13 | 1.0 |