# Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 03:57 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 2MHC |
| BMRB ID | : | 19625 |
| Title | : | NMR structure of the catalytic domain of the large serine resolvase TnpX |
| Authors | : | Headey, S.J.; Sivakumaran, A.; Adams, V.; Rodgers, A.J.W.; Rood, J.I.; Scanlon, M.J.; Wilce, M.C.J. |
| Deposited on | : | 2013-11-20 |

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

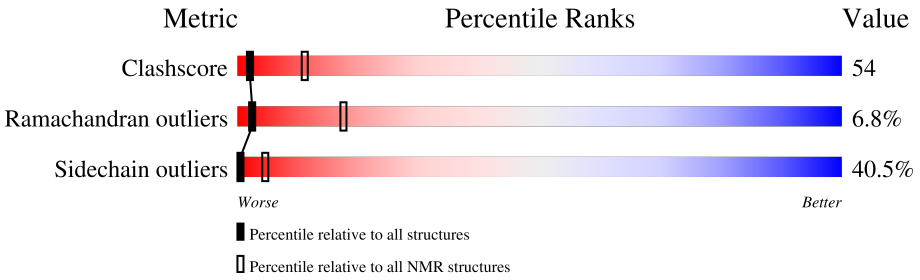
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis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

# 1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 87%.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 120 | 13% 41% 25% 21% |

# 2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 10 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:5-A:13, A:27-A:54, A:60-A:117 (95) | 0.31 | 10 |

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 3 clusters and 1 single-model cluster was found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1917 atoms, of which 944 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TnpX.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 120 | 1917 | 603 | 944 | 177 | 192 | 1 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | GLY | - | expression tag | UNP O05415 |

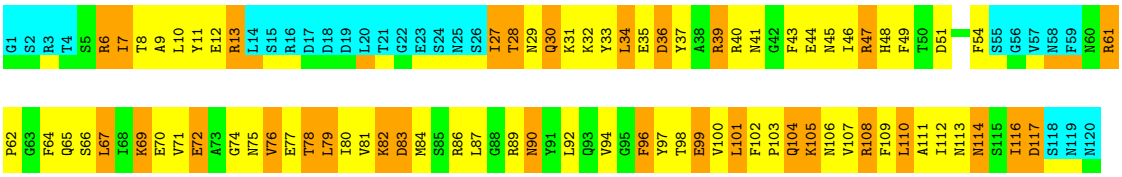
# 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: TnpX

Chain A: 13% 41% 25% 21%



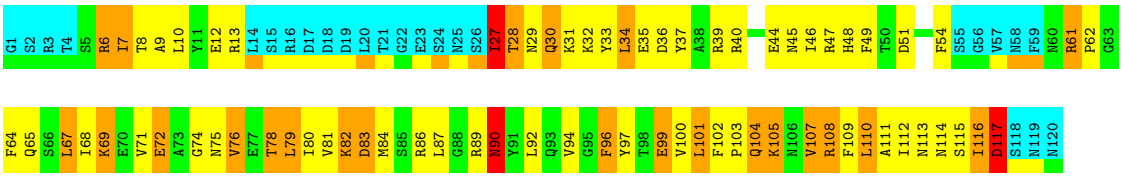

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: TnpX

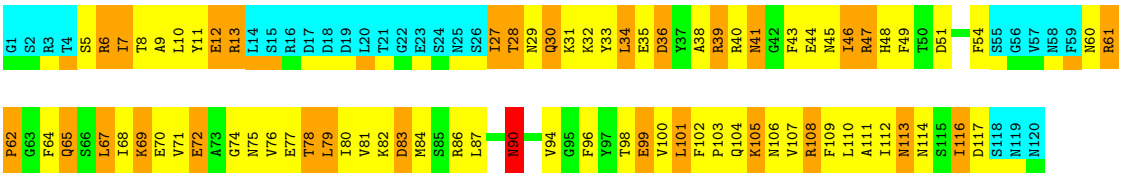
Chain A: 18% 39% 19% • 21%




### 4.2.2 Score per residue for model 2

• Molecule 1: TnpX

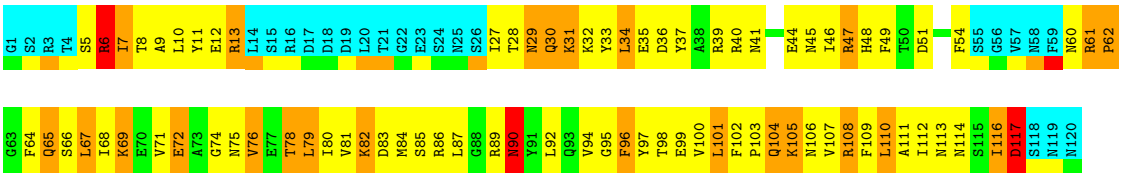
Chain A: 14% 41% 23% • 21%




### 4.2.3 Score per residue for model 3

- Molecule 1: TnpX

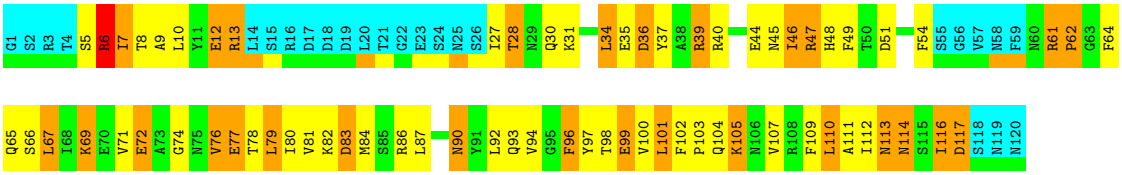
Chain A: 12% 45% 20% • 21%




### 4.2.4 Score per residue for model 4

- Molecule 1: TnpX

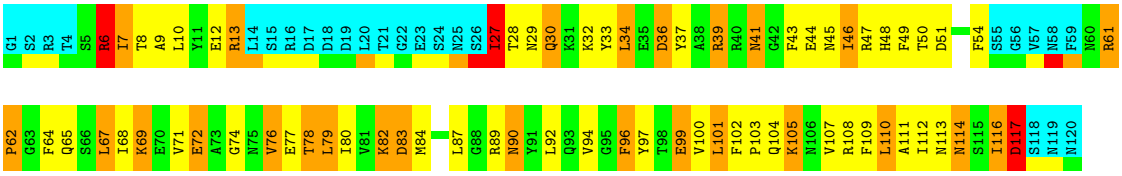
Chain A: 21% 34% 23% • 21%




### 4.2.5 Score per residue for model 5

- Molecule 1: TnpX

Chain A: 21% 34% 22% • 21%




### 4.2.6 Score per residue for model 6

- Molecule 1: TnpX

Chain A: 16% 38% 24% • 21%

G1 S2 R3 T4 S5 R6 I7 T8 A9 L10 Y11 E12 R13 L14 S15 R16 D17 D18 D19 L20 T21 G22 E23 S24 N25 S26 I27 T28 N29 Q30 K31 K32 Y33 L34 E35 D36 Y37 A38 R39 R40 N41 G42 F43 E44 N45 I46 R47 H48 F49 T50 D51 F54 S55 G56 V57 N58 F59 N60 R61

P62 G63 F64 Q65 S66 L67 I68 K69 E70 V71 E72 A73 G74 N75 V76 E77 T78 L79 I80 V81 K82 D83 M84 S85 R86 R89 N90 Y91 L92 Q93 V94 G95 F96 Y97 T98 E99 V100 L101 F102 P103 Q104 K105 N106 V107 R108 F109 L110 A111 I112 N113 N114 S115 I116 D117 S118 N119 N120

### 4.2.7 Score per residue for model 7

- Molecule 1: TnpX

Chain A: 19% 35% 25% 21%

G1 S2 R3 T4 S5 R6 I7 T8 A9 L10 Y11 E12 R13 L14 S15 R16 D17 D18 D19 L20 T21 G22 E23 S24 N25 S26 I27 T28 N29 Q30 K31 K32 Y33 L34 E35 D36 Y37 A38 R39 R40 N41 G42 F43 E44 N45 I46 R47 H48 D51 F54 S55 G56 V57 N58 F59 N60 R61 P62

G63 F64 L67 I68 K69 E70 V71 E72 A73 G74 N75 V76 E77 T78 L79 I80 V81 K82 D83 M84 S85 R86 L87 N90 Y91 L92 F96 Y97 T98 E99 V100 L101 F102 P103 Q104 K105 N106 V107 R108 F109 L110 A111 I112 N113 N114 S115 I116 D117 S118 N119 N120

### 4.2.8 Score per residue for model 8

- Molecule 1: TnpX

Chain A: 18% 34% 26% • 21%

G1 S2 R3 T4 S5 R6 I7 T8 A9 L10 Y11 E12 R13 L14 S15 R16 D17 D18 D19 L20 T21 G22 E23 S24 N25 S26 I27 T28 N29 Q30 K31 L34 E35 D36 Y37 A38 R39 R40 N41 G42 F43 E44 N45 I46 R47 H48 F49 T50 D51 F54 S55 G56 V57 N58 F59 N60 R61 P62

G63 F64 Q65 S66 L67 I68 K69 E70 V71 E72 A73 G74 N75 V76 E77 T78 L79 I80 V81 K82 D83 M84 S85 R86 L87 N90 Y91 L92 Q93 V94 G95 F96 Y97 T98 E99 V100 L101 F102 P103 Q104 K105 N106 V107 R108 F109 L110 A111 I112 N113 N114 S115 I116 D117 S118 N119 N120

### 4.2.9 Score per residue for model 9

- Molecule 1: TnpX

Chain A: 18% 39% 22% 21%

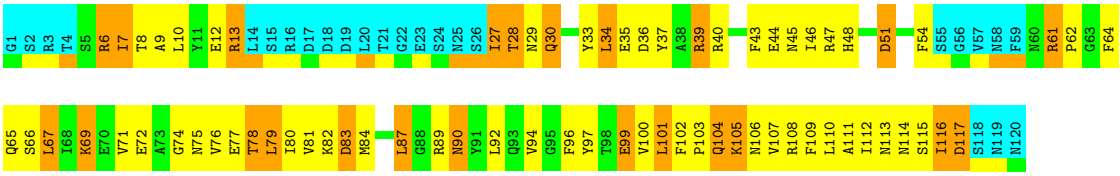
G1 S2 R3 T4 S5 R6 I7 T8 A9 L10 Y11 E12 R13 L14 S15 R16 D17 D18 D19 L20 T21 G22 E23 S24 N25 S26 I27 T28 N29 Q30 K31 K32 Y33 L34 E35 D36 Y37 A38 R39 R40 E44 N45 I46 R47 H48 F49 T50 D51 F54 S55 G56 V57 N58 F59 N60 R61 P62 G63

F64 Q65 S66 L67 I68 K69 E70 V71 E72 A73 G74 N75 V76 E77 T78 L79 I80 V81 K82 D83 R86 L87 G88 R89 N90 Y91 L92 F96 Y97 T98 E99 V100 L101 F102 P103 Q104 K105 N106 V107 R108 F109 L110 A111 I112 N113 N114 S115 I116 D117 S118 N119 N120

### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: TnpX

Chain A: 19% 41% 19% 21%



# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *TORSION ANGLE DYNAMICS, SIMULATED ANNEALING, SIMULATED ANNEALING.*

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *STRUCTURES WITH THE LOWEST ENER.*

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

| **Software name** | **Classification** | **Version** |
|---|---|---|
| CNSSOLVE | refinement | 1.2 |
| XEASY | structure solution | 1.4 |

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 | 1448 |
| Number of shifts mapped to atoms | 1448 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 87% |

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 789 | 781 | 780 | 84±8 |
| All | All | 7890 | 7810 | 7800 | 841 |

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 54.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:71:VAL:HG22 | 1:A:76:VAL:HG11 | 1.05 | 1.22 | 1 | 10 |
| 1:A:71:VAL:HG13 | 1:A:105:LYS:NZ | 0.81 | 1.89 | 6 | 1 |
| 1:A:110:LEU:HD13 | 1:A:111:ALA:N | 0.80 | 1.92 | 10 | 1 |
| 1:A:90:ASN:O | 1:A:94:VAL:HG23 | 0.77 | 1.80 | 1 | 5 |
| 1:A:9:ALA:HB2 | 1:A:76:VAL:HG23 | 0.77 | 1.57 | 8 | 9 |
| 1:A:71:VAL:CG2 | 1:A:76:VAL:HG11 | 0.75 | 2.09 | 1 | 4 |
| 1:A:71:VAL:HA | 1:A:76:VAL:HG12 | 0.74 | 1.58 | 1 | 10 |
| 1:A:102:PHE:CD2 | 1:A:107:VAL:HG21 | 0.73 | 2.18 | 3 | 10 |
| 1:A:61:ARG:HG3 | 1:A:64:PHE:CB | 0.73 | 2.13 | 9 | 4 |
| 1:A:110:LEU:HD22 | 1:A:111:ALA:N | 0.71 | 2.00 | 6 | 9 |
| 1:A:74:GLY:HA2 | 1:A:105:LYS:HG2 | 0.70 | 1.64 | 5 | 10 |
| 1:A:110:LEU:HD11 | 1:A:112:ILE:HG13 | 0.70 | 1.63 | 1 | 8 |
| 1:A:110:LEU:HD11 | 1:A:112:ILE:CD1 | 0.70 | 2.17 | 6 | 2 |
| 1:A:71:VAL:HG22 | 1:A:76:VAL:CG1 | 0.69 | 2.15 | 6 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:34:LEU:HG | 1:A:80:ILE:HG22 | 0.68 | 1.65 | 10 | 7 |
| 1:A:51:ASP:HA | 1:A:54:PHE:CE2 | 0.67 | 2.25 | 5 | 3 |
| 1:A:7:ILE:HD12 | 1:A:8:THR:O | 0.67 | 1.89 | 6 | 8 |
| 1:A:76:VAL:O | 1:A:76:VAL:HG13 | 0.67 | 1.89 | 4 | 10 |
| 1:A:10:LEU:CD2 | 1:A:34:LEU:HD23 | 0.67 | 2.20 | 4 | 4 |
| 1:A:9:ALA:HB2 | 1:A:76:VAL:CG2 | 0.67 | 2.19 | 5 | 10 |
| 1:A:79:LEU:HD12 | 1:A:81:VAL:HG23 | 0.66 | 1.66 | 8 | 9 |
| 1:A:102:PHE:HD2 | 1:A:107:VAL:HG11 | 0.66 | 1.51 | 4 | 10 |
| 1:A:34:LEU:HG | 1:A:80:ILE:CG2 | 0.66 | 2.20 | 10 | 3 |
| 1:A:9:ALA:CB | 1:A:76:VAL:HG23 | 0.65 | 2.21 | 8 | 6 |
| 1:A:10:LEU:HD22 | 1:A:48:HIS:ND1 | 0.65 | 2.05 | 3 | 10 |
| 1:A:13:ARG:HA | 1:A:51:ASP:CG | 0.65 | 2.12 | 8 | 3 |
| 1:A:51:ASP:HB2 | 1:A:54:PHE:CE2 | 0.64 | 2.27 | 10 | 7 |
| 1:A:33:TYR:HE2 | 1:A:112:ILE:HD13 | 0.64 | 1.52 | 5 | 7 |
| 1:A:27:ILE:HA | 1:A:30:GLN:NE2 | 0.63 | 2.08 | 6 | 4 |
| 1:A:67:LEU:O | 1:A:71:VAL:HG23 | 0.63 | 1.94 | 3 | 7 |
| 1:A:102:PHE:CD2 | 1:A:107:VAL:HG11 | 0.63 | 2.28 | 4 | 10 |
| 1:A:61:ARG:CG | 1:A:64:PHE:CB | 0.63 | 2.76 | 3 | 9 |
| 1:A:105:LYS:N | 1:A:105:LYS:HD3 | 0.62 | 2.07 | 3 | 1 |
| 1:A:71:VAL:CG1 | 1:A:101:LEU:HD12 | 0.61 | 2.25 | 3 | 5 |
| 1:A:13:ARG:HA | 1:A:51:ASP:HB2 | 0.61 | 1.71 | 4 | 3 |
| 1:A:13:ARG:NH1 | 1:A:86:ARG:HD3 | 0.61 | 2.10 | 4 | 3 |
| 1:A:51:ASP:CB | 1:A:54:PHE:CE2 | 0.61 | 2.83 | 8 | 7 |
| 1:A:36:ASP:HA | 1:A:39:ARG:HD3 | 0.61 | 1.72 | 6 | 7 |
| 1:A:41:ASN:HB3 | 1:A:43:PHE:CE2 | 0.61 | 2.30 | 7 | 5 |
| 1:A:11:TYR:CE1 | 1:A:86:ARG:HB3 | 0.61 | 2.29 | 8 | 1 |
| 1:A:10:LEU:HD22 | 1:A:48:HIS:CE1 | 0.60 | 2.31 | 1 | 5 |
| 1:A:74:GLY:HA2 | 1:A:105:LYS:CG | 0.60 | 2.27 | 2 | 10 |
| 1:A:34:LEU:N | 1:A:34:LEU:HD13 | 0.60 | 2.11 | 9 | 4 |
| 1:A:74:GLY:CA | 1:A:105:LYS:HG2 | 0.60 | 2.27 | 6 | 10 |
| 1:A:71:VAL:HG13 | 1:A:105:LYS:HZ1 | 0.60 | 1.56 | 6 | 1 |
| 1:A:12:GLU:HG2 | 1:A:30:GLN:HB2 | 0.60 | 1.71 | 1 | 1 |
| 1:A:64:PHE:CD1 | 1:A:67:LEU:HD23 | 0.60 | 2.31 | 8 | 2 |
| 1:A:43:PHE:CE1 | 1:A:78:THR:HG21 | 0.60 | 2.32 | 6 | 3 |
| 1:A:80:ILE:HG23 | 1:A:110:LEU:HD12 | 0.59 | 1.74 | 4 | 2 |
| 1:A:51:ASP:CG | 1:A:54:PHE:CE2 | 0.59 | 2.76 | 3 | 3 |
| 1:A:47:ARG:HD2 | 1:A:49:PHE:CZ | 0.59 | 2.32 | 9 | 3 |
| 1:A:102:PHE:O | 1:A:105:LYS:HE3 | 0.59 | 1.96 | 1 | 4 |
| 1:A:9:ALA:HB3 | 1:A:79:LEU:HD22 | 0.59 | 1.74 | 3 | 7 |
| 1:A:102:PHE:HA | 1:A:105:LYS:NZ | 0.58 | 2.13 | 6 | 1 |
| 1:A:6:ARG:HB2 | 1:A:75:ASN:O | 0.58 | 1.99 | 3 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:47:ARG:HD3 | 1:A:49:PHE:CZ | 0.58 | 2.34 | 3 | 1 |
| 1:A:79:LEU:HG | 1:A:109:PHE:CE2 | 0.58 | 2.33 | 1 | 9 |
| 1:A:13:ARG:HB2 | 1:A:51:ASP:CB | 0.58 | 2.29 | 5 | 1 |
| 1:A:84:MET:SD | 1:A:94:VAL:HG11 | 0.58 | 2.39 | 5 | 5 |
| 1:A:104:GLN:HB2 | 1:A:105:LYS:HD3 | 0.58 | 1.75 | 3 | 1 |
| 1:A:33:TYR:CE2 | 1:A:112:ILE:HD13 | 0.58 | 2.34 | 5 | 7 |
| 1:A:27:ILE:HG22 | 1:A:28:THR:N | 0.57 | 2.13 | 10 | 4 |
| 1:A:11:TYR:CE2 | 1:A:86:ARG:HB3 | 0.57 | 2.34 | 7 | 3 |
| 1:A:71:VAL:HG13 | 1:A:105:LYS:HZ3 | 0.57 | 1.60 | 6 | 2 |
| 1:A:13:ARG:HA | 1:A:51:ASP:HB3 | 0.57 | 1.76 | 6 | 4 |
| 1:A:110:LEU:C | 1:A:110:LEU:HD13 | 0.56 | 2.20 | 8 | 8 |
| 1:A:102:PHE:HD2 | 1:A:107:VAL:HG21 | 0.56 | 1.55 | 3 | 2 |
| 1:A:79:LEU:C | 1:A:80:ILE:HD12 | 0.56 | 2.21 | 6 | 4 |
| 1:A:13:ARG:HB3 | 1:A:86:ARG:CD | 0.56 | 2.31 | 8 | 2 |
| 1:A:96:PHE:CE1 | 1:A:101:LEU:HD23 | 0.56 | 2.36 | 8 | 6 |
| 1:A:69:LYS:O | 1:A:72:GLU:HG3 | 0.55 | 2.01 | 10 | 10 |
| 1:A:61:ARG:HG3 | 1:A:64:PHE:HB2 | 0.55 | 1.78 | 10 | 7 |
| 1:A:102:PHE:N | 1:A:103:PRO:CD | 0.55 | 2.69 | 3 | 10 |
| 1:A:96:PHE:O | 1:A:100:VAL:HG12 | 0.55 | 2.02 | 2 | 8 |
| 1:A:96:PHE:CZ | 1:A:101:LEU:HD23 | 0.55 | 2.37 | 5 | 5 |
| 1:A:54:PHE:CE1 | 1:A:62:PRO:HD2 | 0.55 | 2.37 | 3 | 4 |
| 1:A:9:ALA:CB | 1:A:76:VAL:CG2 | 0.55 | 2.84 | 1 | 7 |
| 1:A:33:TYR:CE2 | 1:A:82:LYS:HE3 | 0.54 | 2.38 | 1 | 4 |
| 1:A:78:THR:HG23 | 1:A:108:ARG:HB3 | 0.54 | 1.78 | 1 | 2 |
| 1:A:12:GLU:HB2 | 1:A:34:LEU:HD21 | 0.54 | 1.78 | 4 | 1 |
| 1:A:51:ASP:HA | 1:A:54:PHE:CZ | 0.53 | 2.38 | 10 | 5 |
| 1:A:13:ARG:HA | 1:A:51:ASP:CB | 0.53 | 2.33 | 6 | 4 |
| 1:A:37:TYR:CD1 | 1:A:38:ALA:N | 0.53 | 2.76 | 8 | 3 |
| 1:A:74:GLY:CA | 1:A:105:LYS:CG | 0.53 | 2.86 | 3 | 1 |
| 1:A:105:LYS:N | 1:A:105:LYS:CD | 0.53 | 2.71 | 3 | 1 |
| 1:A:101:LEU:C | 1:A:103:PRO:HD2 | 0.53 | 2.24 | 4 | 10 |
| 1:A:6:ARG:HG2 | 1:A:7:ILE:N | 0.53 | 2.18 | 5 | 4 |
| 1:A:110:LEU:HD11 | 1:A:112:ILE:CG1 | 0.53 | 2.33 | 8 | 5 |
| 1:A:76:VAL:HG13 | 1:A:105:LYS:NZ | 0.53 | 2.19 | 1 | 3 |
| 1:A:98:THR:HG22 | 1:A:109:PHE:CD2 | 0.53 | 2.38 | 2 | 7 |
| 1:A:74:GLY:C | 1:A:105:LYS:HG2 | 0.52 | 2.25 | 6 | 3 |
| 1:A:111:ALA:HB2 | 1:A:116:ILE:HG12 | 0.52 | 1.82 | 2 | 6 |
| 1:A:71:VAL:HG11 | 1:A:101:LEU:HD12 | 0.52 | 1.81 | 3 | 4 |
| 1:A:36:ASP:HA | 1:A:39:ARG:CD | 0.52 | 2.35 | 9 | 8 |
| 1:A:83:ASP:HB3 | 1:A:113:ASN:HB2 | 0.52 | 1.81 | 2 | 4 |
| 1:A:101:LEU:O | 1:A:104:GLN:HG3 | 0.52 | 2.05 | 1 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:102:PHE:N | 1:A:103:PRO:HD2 | 0.51 | 2.21 | 3 | 10 |
| 1:A:99:GLU:O | 1:A:103:PRO:CG | 0.51 | 2.59 | 3 | 10 |
| 1:A:95:GLY:O | 1:A:99:GLU:N | 0.51 | 2.44 | 3 | 1 |
| 1:A:10:LEU:HD21 | 1:A:34:LEU:HB2 | 0.51 | 1.81 | 5 | 4 |
| 1:A:51:ASP:HB2 | 1:A:54:PHE:CD2 | 0.51 | 2.40 | 2 | 1 |
| 1:A:110:LEU:HD11 | 1:A:112:ILE:HD12 | 0.51 | 1.83 | 6 | 1 |
| 1:A:37:TYR:CZ | 1:A:110:LEU:HG | 0.51 | 2.41 | 1 | 5 |
| 1:A:110:LEU:HD13 | 1:A:110:LEU:O | 0.50 | 2.06 | 8 | 5 |
| 1:A:116:ILE:CG2 | 1:A:117:ASP:N | 0.50 | 2.75 | 1 | 7 |
| 1:A:83:ASP:HB3 | 1:A:113:ASN:CB | 0.50 | 2.35 | 9 | 5 |
| 1:A:84:MET:CE | 1:A:116:ILE:HD11 | 0.50 | 2.36 | 4 | 3 |
| 1:A:10:LEU:HD21 | 1:A:34:LEU:HD23 | 0.50 | 1.82 | 4 | 2 |
| 1:A:7:ILE:HA | 1:A:45:ASN:HB2 | 0.50 | 1.84 | 2 | 9 |
| 1:A:49:PHE:CE1 | 1:A:67:LEU:HA | 0.50 | 2.42 | 3 | 1 |
| 1:A:61:ARG:O | 1:A:65:GLN:N | 0.49 | 2.43 | 5 | 9 |
| 1:A:61:ARG:HG2 | 1:A:64:PHE:CB | 0.49 | 2.37 | 4 | 2 |
| 1:A:110:LEU:HD13 | 1:A:110:LEU:C | 0.49 | 2.26 | 10 | 2 |
| 1:A:102:PHE:HB3 | 1:A:107:VAL:HB | 0.49 | 1.84 | 4 | 10 |
| 1:A:12:GLU:HG2 | 1:A:34:LEU:CD2 | 0.49 | 2.37 | 9 | 2 |
| 1:A:6:ARG:HG3 | 1:A:77:GLU:HB3 | 0.49 | 1.84 | 7 | 3 |
| 1:A:47:ARG:HD2 | 1:A:49:PHE:CE1 | 0.49 | 2.42 | 9 | 1 |
| 1:A:71:VAL:HA | 1:A:76:VAL:CG1 | 0.49 | 2.38 | 4 | 5 |
| 1:A:61:ARG:CG | 1:A:64:PHE:HB3 | 0.49 | 2.36 | 3 | 2 |
| 1:A:76:VAL:O | 1:A:76:VAL:CG1 | 0.49 | 2.61 | 4 | 5 |
| 1:A:69:LYS:HE2 | 1:A:69:LYS:C | 0.48 | 2.29 | 5 | 1 |
| 1:A:27:ILE:O | 1:A:31:LYS:HG3 | 0.48 | 2.08 | 7 | 4 |
| 1:A:92:LEU:HD12 | 1:A:92:LEU:N | 0.48 | 2.23 | 4 | 9 |
| 1:A:78:THR:HG22 | 1:A:108:ARG:O | 0.48 | 2.08 | 7 | 2 |
| 1:A:92:LEU:HD12 | 1:A:92:LEU:H | 0.48 | 1.67 | 8 | 8 |
| 1:A:61:ARG:CG | 1:A:64:PHE:HB2 | 0.48 | 2.39 | 4 | 2 |
| 1:A:37:TYR:HA | 1:A:40:ARG:HG2 | 0.48 | 1.83 | 6 | 1 |
| 1:A:61:ARG:HG3 | 1:A:64:PHE:CG | 0.48 | 2.44 | 9 | 1 |
| 1:A:10:LEU:HD11 | 1:A:34:LEU:HB3 | 0.48 | 1.86 | 2 | 1 |
| 1:A:12:GLU:CD | 1:A:12:GLU:N | 0.48 | 2.67 | 2 | 1 |
| 1:A:49:PHE:CE2 | 1:A:67:LEU:HA | 0.47 | 2.44 | 8 | 1 |
| 1:A:10:LEU:HD13 | 1:A:46:ILE:CG2 | 0.47 | 2.40 | 6 | 2 |
| 1:A:11:TYR:HD1 | 1:A:81:VAL:HG22 | 0.47 | 1.69 | 8 | 1 |
| 1:A:81:VAL:CG1 | 1:A:86:ARG:HG3 | 0.47 | 2.39 | 6 | 2 |
| 1:A:37:TYR:O | 1:A:40:ARG:HG2 | 0.47 | 2.09 | 10 | 5 |
| 1:A:6:ARG:HB3 | 1:A:75:ASN:O | 0.47 | 2.10 | 2 | 1 |
| 1:A:47:ARG:HD3 | 1:A:49:PHE:CE1 | 0.47 | 2.44 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:51:ASP:CG | 1:A:54:PHE:HE2 | 0.47 | 2.12 | 4 | 2 |
| 1:A:96:PHE:CD2 | 1:A:100:VAL:CG1 | 0.47 | 2.98 | 8 | 7 |
| 1:A:11:TYR:CE2 | 1:A:87:LEU:HD12 | 0.47 | 2.45 | 7 | 1 |
| 1:A:110:LEU:CD1 | 1:A:112:ILE:HG13 | 0.47 | 2.39 | 10 | 1 |
| 1:A:97:TYR:O | 1:A:102:PHE:CD1 | 0.47 | 2.68 | 8 | 9 |
| 1:A:34:LEU:HD13 | 1:A:34:LEU:H | 0.47 | 1.68 | 9 | 1 |
| 1:A:81:VAL:HG12 | 1:A:83:ASP:H | 0.47 | 1.68 | 9 | 1 |
| 1:A:9:ALA:CB | 1:A:79:LEU:HD22 | 0.47 | 2.40 | 7 | 5 |
| 1:A:104:GLN:CB | 1:A:105:LYS:HD3 | 0.47 | 2.40 | 3 | 1 |
| 1:A:104:GLN:C | 1:A:105:LYS:HD3 | 0.46 | 2.31 | 3 | 1 |
| 1:A:84:MET:CE | 1:A:109:PHE:CE1 | 0.46 | 2.99 | 3 | 4 |
| 1:A:61:ARG:HG3 | 1:A:64:PHE:HB3 | 0.46 | 1.87 | 8 | 1 |
| 1:A:74:GLY:HA2 | 1:A:105:LYS:CD | 0.46 | 2.40 | 3 | 1 |
| 1:A:34:LEU:N | 1:A:34:LEU:CD1 | 0.46 | 2.77 | 9 | 4 |
| 1:A:74:GLY:HA2 | 1:A:105:LYS:HD2 | 0.46 | 1.86 | 3 | 1 |
| 1:A:49:PHE:CZ | 1:A:67:LEU:HA | 0.46 | 2.46 | 5 | 4 |
| 1:A:80:ILE:HD12 | 1:A:80:ILE:N | 0.46 | 2.25 | 6 | 3 |
| 1:A:110:LEU:O | 1:A:110:LEU:HD13 | 0.46 | 2.10 | 6 | 1 |
| 1:A:12:GLU:CG | 1:A:34:LEU:CD2 | 0.46 | 2.94 | 9 | 2 |
| 1:A:78:THR:HG23 | 1:A:108:ARG:CB | 0.46 | 2.40 | 2 | 4 |
| 1:A:98:THR:CG2 | 1:A:109:PHE:CD2 | 0.45 | 2.99 | 2 | 2 |
| 1:A:83:ASP:HB3 | 1:A:113:ASN:HB3 | 0.45 | 1.87 | 10 | 3 |
| 1:A:51:ASP:CA | 1:A:54:PHE:CE2 | 0.45 | 3.00 | 4 | 2 |
| 1:A:84:MET:HE1 | 1:A:116:ILE:HD11 | 0.45 | 1.89 | 6 | 1 |
| 1:A:79:LEU:HD13 | 1:A:80:ILE:N | 0.45 | 2.26 | 8 | 1 |
| 1:A:30:GLN:O | 1:A:33:TYR:HB3 | 0.45 | 2.11 | 5 | 3 |
| 1:A:38:ALA:CB | 1:A:46:ILE:HD13 | 0.45 | 2.42 | 2 | 1 |
| 1:A:28:THR:HA | 1:A:31:LYS:HG3 | 0.45 | 1.89 | 2 | 3 |
| 1:A:30:GLN:OE1 | 1:A:31:LYS:HG2 | 0.45 | 2.12 | 8 | 3 |
| 1:A:47:ARG:CD | 1:A:49:PHE:CE1 | 0.45 | 3.00 | 2 | 1 |
| 1:A:69:LYS:HA | 1:A:72:GLU:CG | 0.45 | 2.42 | 4 | 4 |
| 1:A:111:ALA:CB | 1:A:116:ILE:HG12 | 0.45 | 2.42 | 4 | 2 |
| 1:A:102:PHE:O | 1:A:105:LYS:CE | 0.45 | 2.64 | 5 | 1 |
| 1:A:11:TYR:HD2 | 1:A:81:VAL:HG22 | 0.45 | 1.71 | 7 | 1 |
| 1:A:54:PHE:CE1 | 1:A:61:ARG:HB3 | 0.44 | 2.47 | 3 | 2 |
| 1:A:10:LEU:HD11 | 1:A:34:LEU:CB | 0.44 | 2.42 | 4 | 2 |
| 1:A:97:TYR:HA | 1:A:101:LEU:CB | 0.44 | 2.42 | 6 | 2 |
| 1:A:37:TYR:CD1 | 1:A:80:ILE:HG12 | 0.44 | 2.47 | 10 | 1 |
| 1:A:68:ILE:O | 1:A:72:GLU:HG2 | 0.44 | 2.12 | 2 | 4 |
| 1:A:71:VAL:CA | 1:A:76:VAL:HG12 | 0.44 | 2.40 | 8 | 2 |
| 1:A:69:LYS:HG3 | 1:A:70:GLU:N | 0.44 | 2.27 | 8 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:78:THR:HG22 | 1:A:108:ARG:HB3 | 0.44 | 1.88 | 8 | 1 |
| 1:A:7:ILE:HG23 | 1:A:75:ASN:HB3 | 0.44 | 1.89 | 2 | 1 |
| 1:A:27:ILE:HG22 | 1:A:31:LYS:HE2 | 0.44 | 1.90 | 3 | 1 |
| 1:A:33:TYR:CE2 | 1:A:82:LYS:CE | 0.44 | 3.01 | 9 | 4 |
| 1:A:100:VAL:C | 1:A:103:PRO:HD2 | 0.44 | 2.33 | 9 | 8 |
| 1:A:12:GLU:HB2 | 1:A:34:LEU:CD2 | 0.44 | 2.42 | 5 | 1 |
| 1:A:104:GLN:HB2 | 1:A:105:LYS:HE2 | 0.44 | 1.90 | 7 | 4 |
| 1:A:96:PHE:CD2 | 1:A:100:VAL:HG11 | 0.43 | 2.48 | 8 | 3 |
| 1:A:36:ASP:O | 1:A:39:ARG:HG2 | 0.43 | 2.13 | 3 | 1 |
| 1:A:11:TYR:CE2 | 1:A:86:ARG:NH2 | 0.43 | 2.86 | 8 | 1 |
| 1:A:79:LEU:CD1 | 1:A:81:VAL:HG23 | 0.43 | 2.38 | 8 | 2 |
| 1:A:102:PHE:HA | 1:A:105:LYS:HZ1 | 0.43 | 1.72 | 6 | 1 |
| 1:A:7:ILE:HG12 | 1:A:70:GLU:HG2 | 0.43 | 1.91 | 8 | 1 |
| 1:A:71:VAL:HG12 | 1:A:104:GLN:NE2 | 0.43 | 2.28 | 8 | 1 |
| 1:A:101:LEU:O | 1:A:104:GLN:CG | 0.43 | 2.66 | 8 | 1 |
| 1:A:10:LEU:HD22 | 1:A:48:HIS:CG | 0.43 | 2.48 | 4 | 2 |
| 1:A:38:ALA:HB1 | 1:A:46:ILE:CD1 | 0.43 | 2.44 | 2 | 2 |
| 1:A:34:LEU:HB3 | 1:A:80:ILE:HG21 | 0.43 | 1.90 | 8 | 2 |
| 1:A:84:MET:HE3 | 1:A:109:PHE:CE1 | 0.43 | 2.48 | 3 | 1 |
| 1:A:66:SER:O | 1:A:70:GLU:HG2 | 0.43 | 2.13 | 9 | 1 |
| 1:A:36:ASP:HA | 1:A:39:ARG:NE | 0.43 | 2.29 | 1 | 1 |
| 1:A:45:ASN:O | 1:A:46:ILE:C | 0.43 | 2.57 | 5 | 1 |
| 1:A:97:TYR:HA | 1:A:101:LEU:HB2 | 0.43 | 1.90 | 6 | 1 |
| 1:A:99:GLU:O | 1:A:103:PRO:HG3 | 0.43 | 2.13 | 5 | 4 |
| 1:A:13:ARG:HB3 | 1:A:86:ARG:HD3 | 0.43 | 1.91 | 8 | 1 |
| 1:A:96:PHE:O | 1:A:100:VAL:CG1 | 0.43 | 2.67 | 3 | 1 |
| 1:A:12:GLU:CB | 1:A:34:LEU:HD21 | 0.43 | 2.43 | 4 | 1 |
| 1:A:96:PHE:CD1 | 1:A:96:PHE:C | 0.43 | 2.93 | 9 | 2 |
| 1:A:79:LEU:HD12 | 1:A:81:VAL:CG2 | 0.42 | 2.43 | 2 | 1 |
| 1:A:36:ASP:CA | 1:A:39:ARG:HD3 | 0.42 | 2.44 | 9 | 2 |
| 1:A:12:GLU:O | 1:A:51:ASP:HB3 | 0.42 | 2.14 | 7 | 1 |
| 1:A:110:LEU:C | 1:A:110:LEU:CD1 | 0.42 | 2.87 | 10 | 1 |
| 1:A:82:LYS:O | 1:A:113:ASN:N | 0.42 | 2.52 | 3 | 1 |
| 1:A:99:GLU:O | 1:A:103:PRO:HG2 | 0.42 | 2.14 | 10 | 3 |
| 1:A:102:PHE:HB3 | 1:A:107:VAL:CG1 | 0.42 | 2.44 | 8 | 2 |
| 1:A:12:GLU:CG | 1:A:34:LEU:HD21 | 0.42 | 2.45 | 4 | 1 |
| 1:A:12:GLU:CG | 1:A:30:GLN:HB2 | 0.42 | 2.44 | 1 | 1 |
| 1:A:102:PHE:O | 1:A:105:LYS:HD2 | 0.42 | 2.14 | 7 | 3 |
| 1:A:83:ASP:CB | 1:A:113:ASN:HB3 | 0.42 | 2.45 | 8 | 1 |
| 1:A:64:PHE:C | 1:A:64:PHE:CD1 | 0.42 | 2.92 | 5 | 1 |
| 1:A:11:TYR:CZ | 1:A:86:ARG:HB3 | 0.41 | 2.50 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:36:ASP:HA | 1:A:39:ARG:CZ | 0.41 | 2.45 | 1 | 1 |
| 1:A:109:PHE:CD1 | 1:A:116:ILE:HD11 | 0.41 | 2.51 | 9 | 1 |
| 1:A:13:ARG:CA | 1:A:51:ASP:HB2 | 0.41 | 2.44 | 5 | 1 |
| 1:A:110:LEU:HD12 | 1:A:112:ILE:HG13 | 0.41 | 1.92 | 10 | 1 |
| 1:A:76:VAL:HG13 | 1:A:105:LYS:HZ2 | 0.41 | 1.76 | 1 | 1 |
| 1:A:64:PHE:CD1 | 1:A:64:PHE:C | 0.41 | 2.94 | 2 | 1 |
| 1:A:76:VAL:CG1 | 1:A:76:VAL:O | 0.41 | 2.69 | 6 | 2 |
| 1:A:35:GLU:HG3 | 1:A:48:HIS:NE2 | 0.41 | 2.31 | 2 | 1 |
| 1:A:13:ARG:HA | 1:A:51:ASP:OD1 | 0.41 | 2.15 | 8 | 1 |
| 1:A:12:GLU:HG3 | 1:A:34:LEU:HD21 | 0.41 | 1.93 | 4 | 1 |
| 1:A:79:LEU:CD1 | 1:A:80:ILE:N | 0.41 | 2.84 | 10 | 3 |
| 1:A:61:ARG:CB | 1:A:64:PHE:HB3 | 0.41 | 2.46 | 9 | 1 |
| 1:A:93:GLN:NE2 | 1:A:93:GLN:HA | 0.41 | 2.30 | 4 | 1 |
| 1:A:7:ILE:HG12 | 1:A:70:GLU:CG | 0.41 | 2.46 | 6 | 1 |
| 1:A:11:TYR:CE2 | 1:A:87:LEU:CD1 | 0.41 | 3.04 | 7 | 1 |
| 1:A:11:TYR:HE2 | 1:A:86:ARG:HB3 | 0.40 | 1.71 | 7 | 1 |
| 1:A:10:LEU:HD21 | 1:A:34:LEU:CD2 | 0.40 | 2.47 | 4 | 1 |
| 1:A:67:LEU:HG | 1:A:68:ILE:N | 0.40 | 2.32 | 1 | 1 |
| 1:A:41:ASN:CB | 1:A:43:PHE:CE2 | 0.40 | 3.02 | 7 | 1 |
| 1:A:82:LYS:O | 1:A:112:ILE:HB | 0.40 | 2.17 | 7 | 1 |
| 1:A:35:GLU:C | 1:A:39:ARG:HD3 | 0.40 | 2.37 | 9 | 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 | 95/120 (79%) | 77±2 (81±2%) | 12±3 (12±3%) | 6±1 (7±2%) | 2 17 |
| All | All | 950/1200 (79%) | 770 (81%) | 115 (12%) | 65 (7%) | 2 17 |

All 11 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 | 46 | ILE | 10 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 62 | PRO | 10 |
| 1 | A | 117 | ASP | 9 |
| 1 | A | 76 | VAL | 7 |
| 1 | A | 106 | ASN | 6 |
| 1 | A | 114 | ASN | 6 |
| 1 | A | 27 | ILE | 5 |
| 1 | A | 90 | ASN | 5 |
| 1 | A | 6 | ARG | 4 |
| 1 | A | 60 | ASN | 2 |
| 1 | A | 5 | SER | 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 | 85/107 (79%) | 51±2 (60±2%) | 34±2 (40±2%) | 0 4 |
| All | All | 850/1070 (79%) | 506 (60%) | 344 (40%) | 0 4 |

All 54 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 | 6 | ARG | 10 |
| 1 | A | 7 | ILE | 10 |
| 1 | A | 28 | THR | 10 |
| 1 | A | 30 | GLN | 10 |
| 1 | A | 34 | LEU | 10 |
| 1 | A | 44 | GLU | 10 |
| 1 | A | 47 | ARG | 10 |
| 1 | A | 61 | ARG | 10 |
| 1 | A | 67 | LEU | 10 |
| 1 | A | 69 | LYS | 10 |
| 1 | A | 78 | THR | 10 |
| 1 | A | 79 | LEU | 10 |
| 1 | A | 82 | LYS | 10 |
| 1 | A | 90 | ASN | 10 |
| 1 | A | 101 | LEU | 10 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 105 | LYS | 10 |
| 1 | A | 116 | ILE | 10 |
| 1 | A | 72 | GLU | 9 |
| 1 | A | 99 | GLU | 9 |
| 1 | A | 114 | ASN | 9 |
| 1 | A | 13 | ARG | 9 |
| 1 | A | 96 | PHE | 8 |
| 1 | A | 108 | ARG | 8 |
| 1 | A | 110 | LEU | 8 |
| 1 | A | 39 | ARG | 8 |
| 1 | A | 83 | ASP | 7 |
| 1 | A | 117 | ASP | 7 |
| 1 | A | 12 | GLU | 7 |
| 1 | A | 77 | GLU | 7 |
| 1 | A | 32 | LYS | 6 |
| 1 | A | 35 | GLU | 6 |
| 1 | A | 89 | ARG | 6 |
| 1 | A | 104 | GLN | 6 |
| 1 | A | 36 | ASP | 5 |
| 1 | A | 66 | SER | 5 |
| 1 | A | 41 | ASN | 4 |
| 1 | A | 31 | LYS | 4 |
| 1 | A | 51 | ASP | 4 |
| 1 | A | 115 | SER | 3 |
| 1 | A | 40 | ARG | 3 |
| 1 | A | 65 | GLN | 3 |
| 1 | A | 70 | GLU | 3 |
| 1 | A | 113 | ASN | 3 |
| 1 | A | 11 | TYR | 3 |
| 1 | A | 27 | ILE | 2 |
| 1 | A | 5 | SER | 2 |
| 1 | A | 29 | ASN | 2 |
| 1 | A | 10 | LEU | 2 |
| 1 | A | 107 | VAL | 1 |
| 1 | A | 85 | SER | 1 |
| 1 | A | 50 | THR | 1 |
| 1 | A | 68 | ILE | 1 |
| 1 | A | 86 | ARG | 1 |
| 1 | A | 87 | LEU | 1 |

#### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry (i)

There are no ligands in this entry.

### 6.7 Other polymers (i)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 87% for the entire structure.

## 7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

### 7.1.1 Bookkeeping (i)

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

| | |
|---|---|
| Total number of shifts | 1448 |
| Number of shifts mapped to atoms | 1448 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 3 |

### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 119 | -1.12 ± 0.11 | Should be applied |
| $^{13}C_{\beta}$ | 111 | -0.81 ± 0.15 | Should be applied |
| $^{13}C'$ | 112 | 0.27 ± 0.13 | None needed (< 0.5 ppm) |
| $^{15}N$ | 116 | -0.02 ± 0.36 | None needed (< 0.5 ppm) |

### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1201 atoms were assigned a chemical shift out of a possible 1379. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 472/477 (99%) | 194/194 (100%) | 185/190 (97%) | 93/93 (100%) |
| Sidechain | 657/779 (84%) | 445/499 (89%) | 201/235 (86%) | 11/45 (24%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 72/123 (59%) | 49/59 (83%) | 23/62 (37%) | 0/2 (0%) |
| Overall | 1201/1379 (87%) | 688/752 (91%) | 409/487 (84%) | 104/140 (74%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1448 atoms were assigned a chemical shift out of a possible 1669. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 590/605 (98%) | 243/247 (98%) | 231/240 (96%) | 116/118 (98%) |
| Sidechain | 780/931 (84%) | 528/594 (89%) | 238/282 (84%) | 14/55 (25%) |
| Aromatic | 78/133 (59%) | 53/64 (83%) | 25/67 (37%) | 0/2 (0%) |
| Overall | 1448/1669 (87%) | 824/905 (91%) | 494/589 (84%) | 130/175 (74%) |

### 7.1.4 Statistically unusual chemical shifts (i)

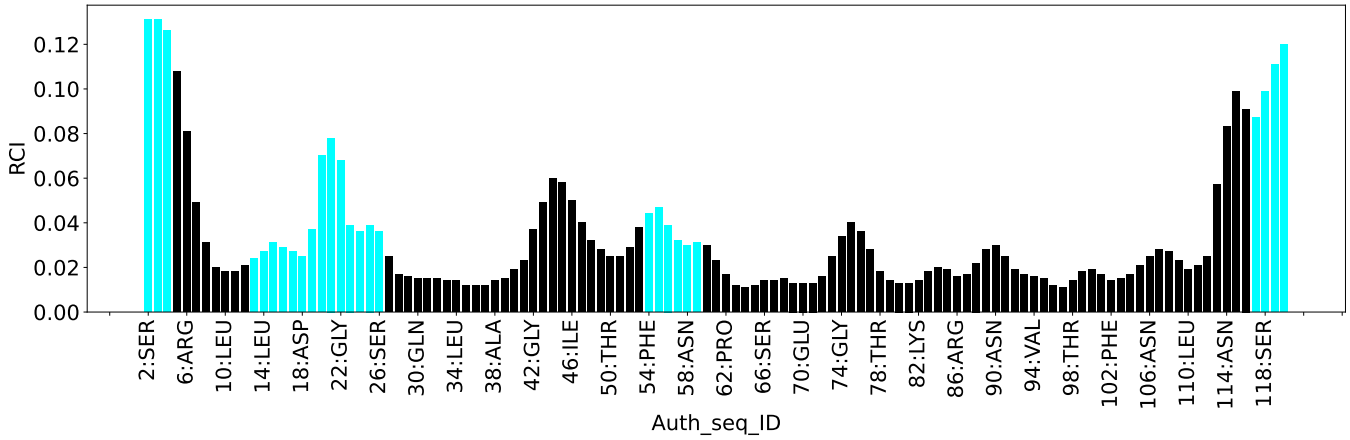
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, *ppm* | Expected range, *ppm* | Z-score |
|---|---|---|---|---|---|---|---|
| 1 | A | 6 | ARG | NE | 98.36 | 76.53 – 92.65 | 8.5 |
| 1 | A | 31 | LYS | HE2 | 1.74 | 1.95 – 3.88 | -6.1 |
| 1 | A | 43 | PHE | CE1 | 138.48 | 124.17 – 137.29 | 5.9 |

### 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
0.00
0.02
0.04
0.06
0.08
0.10
0.12
2:SER
6:ARG
10:LEU
14:LEU
18:ASP
22:GLY
26:SER
30:GLN
34:LEU
38:ALA
42:GLY
46:ILE
50:THR
54:PHE
58:ASN
62:PRO
66:SER
70:GLU
74:GLY
78:THR
82:LYS
86:ARG
90:ASN
94:VAL
98:THR
102:PHE
106:ASN
110:LEU
114:ASN
118:SER
Auth_seq_ID

# 8 NMR restraints analysis (i)

## 8.1 Conformationally restricting restraints (i)

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

| Description | Value |
|---|---|
| Total distance restraints | 1931 |
| Intra-residue (\|i-j\|=0) | 525 |
| Sequential (\|i-j\|=1) | 499 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 333 |
| Long range (\|i-j\|≥5) | 574 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 16.1 |
| Number of long range restraints per residue[1] | 4.8 |

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

## 8.2 Residual restraint violations (i)

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

### 8.2.1 Average number of distance violations per model (i)

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

| Bins (Å) | Average number of violations per model | Max (Å) |
|---|---|---|
| 0.1-0.2 (Small) | 87.2 | 0.2 |
| 0.2-0.5 (Medium) | 9.9 | 0.3 |
| >0.5 (Large) | None | None |

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

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

# 9 Distance violation analysis (i)

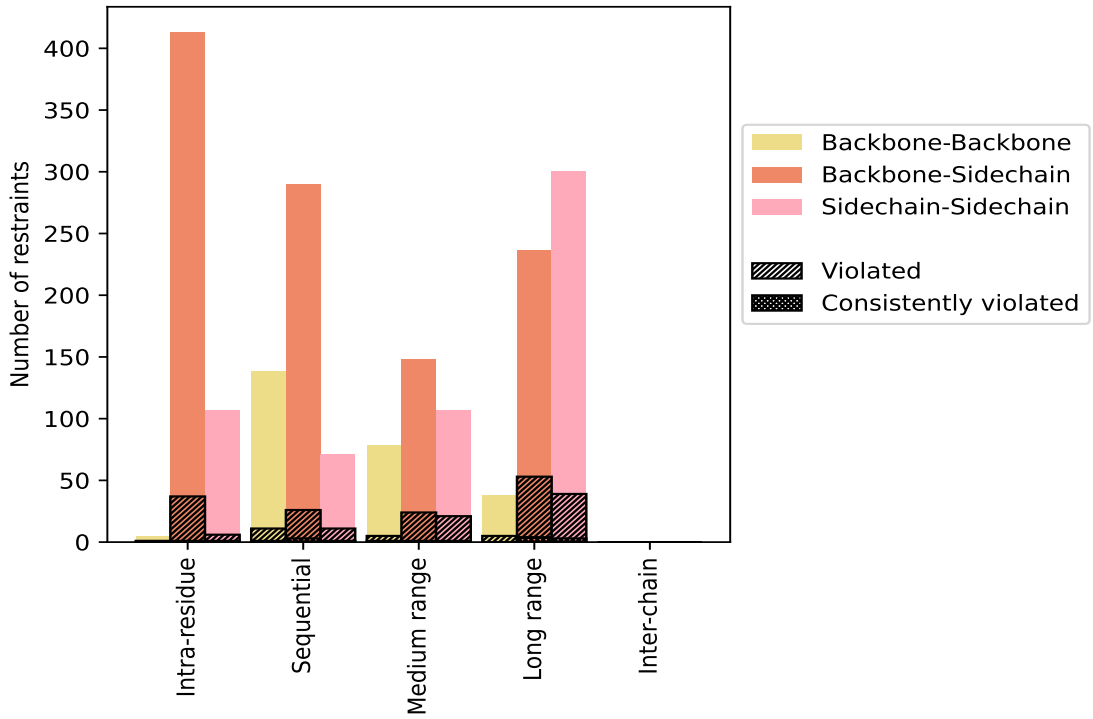
## 9.1 Summary of distance violations (i)

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

| Restraints type | Count | %[1] | Violated[3] | | | Consistently Violated[4] | | |
|---|---|---|---|---|---|---|---|---|
| | | | Count | %[2] | %[1] | Count | %[2] | %[1] |
| Intra-residue (\|i-j\|=0) | 525 | 27.2 | 44 | 8.4 | 2.3 | 2 | 0.4 | 0.1 |
| Backbone-Backbone | 5 | 0.3 | 1 | 20.0 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 413 | 21.4 | 37 | 9.0 | 1.9 | 1 | 0.2 | 0.1 |
| Sidechain-Sidechain | 107 | 5.5 | 6 | 5.6 | 0.3 | 1 | 0.9 | 0.1 |
| Sequential (\|i-j\|=1) | 499 | 25.8 | 48 | 9.6 | 2.5 | 5 | 1.0 | 0.3 |
| Backbone-Backbone | 138 | 7.1 | 11 | 8.0 | 0.6 | 1 | 0.7 | 0.1 |
| Backbone-Sidechain | 290 | 15.0 | 26 | 9.0 | 1.3 | 3 | 1.0 | 0.2 |
| Sidechain-Sidechain | 71 | 3.7 | 11 | 15.5 | 0.6 | 1 | 1.4 | 0.1 |
| Medium range (\|i-j\|>1 & \|i-j\|<5) | 333 | 17.2 | 50 | 15.0 | 2.6 | 3 | 0.9 | 0.2 |
| Backbone-Backbone | 78 | 4.0 | 5 | 6.4 | 0.3 | 1 | 1.3 | 0.1 |
| Backbone-Sidechain | 148 | 7.7 | 24 | 16.2 | 1.2 | 1 | 0.7 | 0.1 |
| Sidechain-Sidechain | 107 | 5.5 | 21 | 19.6 | 1.1 | 1 | 0.9 | 0.1 |
| Long range (\|i-j\|≥5) | 574 | 29.7 | 97 | 16.9 | 5.0 | 7 | 1.2 | 0.4 |
| Backbone-Backbone | 38 | 2.0 | 5 | 13.2 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 236 | 12.2 | 53 | 22.5 | 2.7 | 4 | 1.7 | 0.2 |
| Sidechain-Sidechain | 300 | 15.5 | 39 | 13.0 | 2.0 | 3 | 1.0 | 0.2 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 1931 | 100.0 | 239 | 12.4 | 12.4 | 17 | 0.9 | 0.9 |
| Backbone-Backbone | 259 | 13.4 | 22 | 8.5 | 1.1 | 2 | 0.8 | 0.1 |
| Backbone-Sidechain | 1087 | 56.3 | 140 | 12.9 | 7.3 | 9 | 0.8 | 0.5 |
| Sidechain-Sidechain | 585 | 30.3 | 77 | 13.2 | 4.0 | 6 | 1.0 | 0.3 |

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

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




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

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

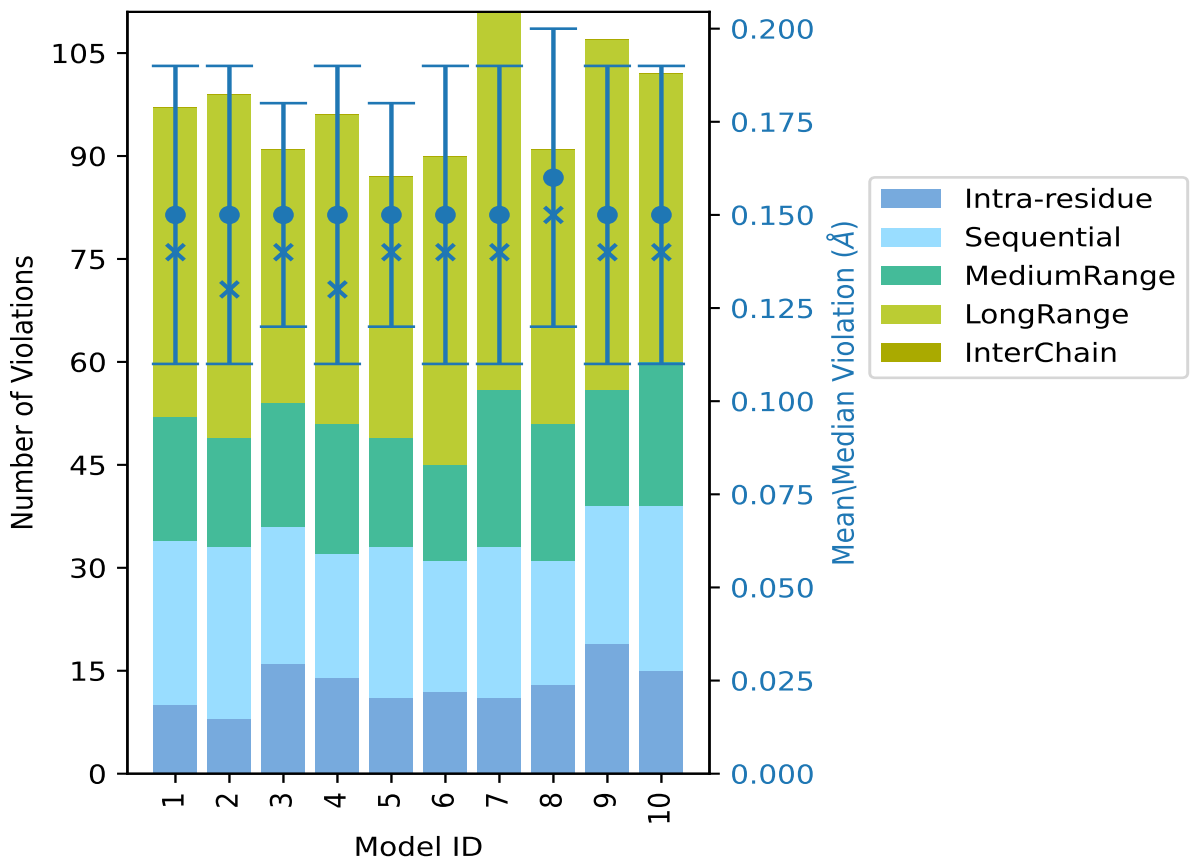
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 1 | 10 | 24 | 18 | 45 | 0 | 97 | 0.15 | 0.27 | 0.04 | 0.14 |
| 2 | 8 | 25 | 16 | 50 | 0 | 99 | 0.15 | 0.26 | 0.04 | 0.13 |
| 3 | 16 | 20 | 18 | 37 | 0 | 91 | 0.15 | 0.29 | 0.03 | 0.14 |
| 4 | 14 | 18 | 19 | 45 | 0 | 96 | 0.15 | 0.27 | 0.04 | 0.13 |
| 5 | 11 | 22 | 16 | 38 | 0 | 87 | 0.15 | 0.24 | 0.03 | 0.14 |
| 6 | 12 | 19 | 14 | 45 | 0 | 90 | 0.15 | 0.29 | 0.04 | 0.14 |
| 7 | 11 | 22 | 23 | 55 | 0 | 111 | 0.15 | 0.3 | 0.04 | 0.14 |
| 8 | 13 | 18 | 20 | 40 | 0 | 91 | 0.16 | 0.28 | 0.04 | 0.15 |
| 9 | 19 | 20 | 17 | 51 | 0 | 107 | 0.15 | 0.27 | 0.04 | 0.14 |
| 10 | 15 | 24 | 21 | 42 | 0 | 102 | 0.15 | 0.28 | 0.04 | 0.14 |

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints,

[5]Inter-chain restraints, [6]Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model (i)




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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1692(IR:481, SQ:451, MR:283, LR:477, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|---|---|---|---|---|---|---|---|
| IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | Count[6] | % |
| 17 | 13 | 16 | 15 | 0 | 61 | 1 | 10.0 |
| 7 | 9 | 8 | 15 | 0 | 39 | 2 | 20.0 |
| 6 | 3 | 6 | 15 | 0 | 30 | 3 | 30.0 |
| 6 | 1 | 4 | 8 | 0 | 19 | 4 | 40.0 |

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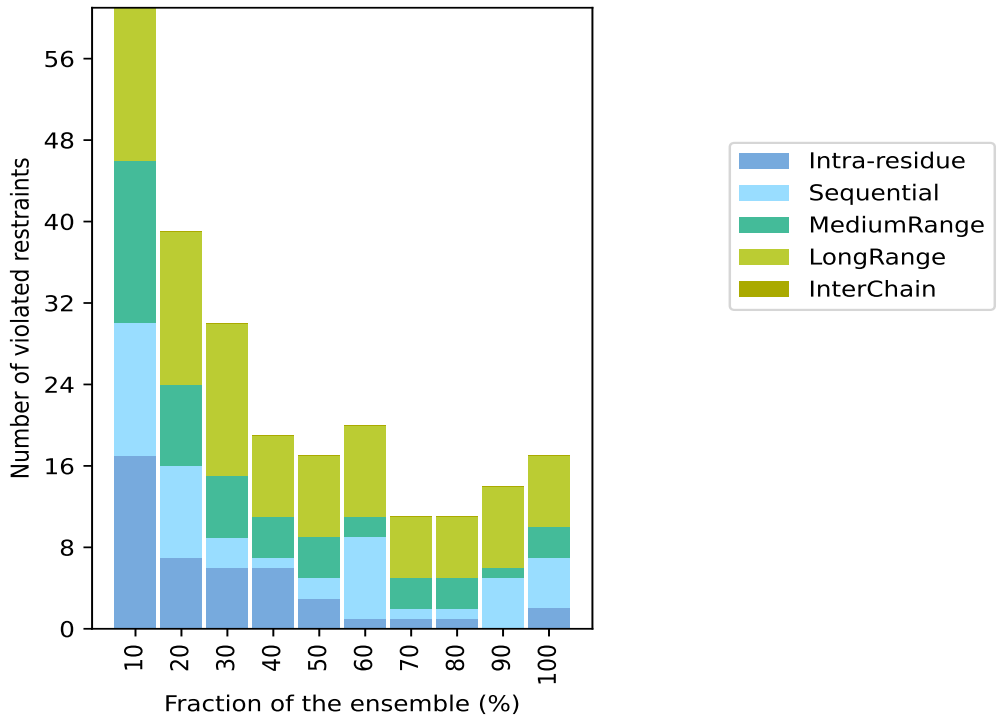
| Number of violated restraints | | | | | | Fraction of the ensemble | |
|---|---|---|---|---|---|---|---|
| IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | Count[6] | % |
| 3 | 2 | 4 | 8 | 0 | 17 | 5 | 50.0 |
| 1 | 8 | 2 | 9 | 0 | 20 | 6 | 60.0 |
| 1 | 1 | 3 | 6 | 0 | 11 | 7 | 70.0 |
| 1 | 1 | 3 | 6 | 0 | 11 | 8 | 80.0 |
| 0 | 5 | 1 | 8 | 0 | 14 | 9 | 90.0 |
| 2 | 5 | 3 | 7 | 0 | 17 | 10 | 100.0 |

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

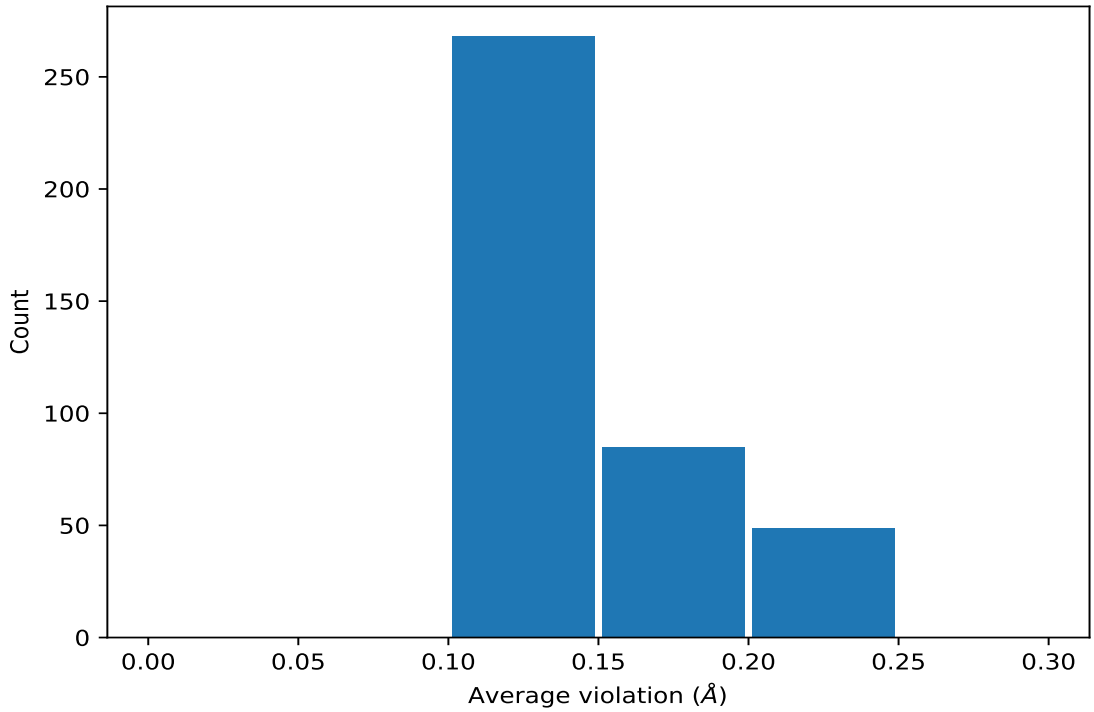
### 9.3.1 Bar graph : Distance violation statistics for the ensemble (i)




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

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

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




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

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

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 10 | 0.24 | 0.03 | 0.24 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 10 | 0.24 | 0.04 | 0.26 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 10 | 0.24 | 0.03 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 10 | 0.24 | 0.03 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 10 | 0.24 | 0.03 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 10 | 0.24 | 0.03 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 10 | 0.24 | 0.03 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 10 | 0.24 | 0.03 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 10 | 0.24 | 0.03 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 10 | 0.24 | 0.03 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 10 | 0.24 | 0.03 | 0.23 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 10 | 0.2 | 0.03 | 0.2 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 10 | 0.19 | 0.04 | 0.2 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 10 | 0.19 | 0.04 | 0.2 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 10 | 0.17 | 0.02 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 10 | 0.17 | 0.03 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 10 | 0.17 | 0.03 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 10 | 0.17 | 0.03 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 10 | 0.17 | 0.03 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 10 | 0.17 | 0.03 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 10 | 0.17 | 0.03 | 0.18 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 10 | 0.16 | 0.03 | 0.15 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 10 | 0.15 | 0.02 | 0.15 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 10 | 0.15 | 0.02 | 0.15 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 10 | 0.15 | 0.02 | 0.15 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 10 | 0.15 | 0.04 | 0.14 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 10 | 0.14 | 0.02 | 0.14 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 10 | 0.14 | 0.02 | 0.14 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 10 | 0.14 | 0.02 | 0.14 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 10 | 0.14 | 0.01 | 0.14 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 10 | 0.13 | 0.02 | 0.13 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 10 | 0.13 | 0.01 | 0.13 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 10 | 0.12 | 0.01 | 0.12 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 9 | 0.21 | 0.03 | 0.2 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 9 | 0.2 | 0.03 | 0.21 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 9 | 0.2 | 0.03 | 0.2 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 9 | 0.2 | 0.03 | 0.19 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 9 | 0.2 | 0.03 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 9 | 0.19 | 0.02 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 9 | 0.19 | 0.02 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 9 | 0.19 | 0.02 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 9 | 0.19 | 0.02 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 9 | 0.19 | 0.02 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 9 | 0.19 | 0.02 | 0.2 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 9 | 0.18 | 0.04 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 9 | 0.18 | 0.04 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 9 | 0.18 | 0.04 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 9 | 0.17 | 0.04 | 0.16 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 9 | 0.17 | 0.04 | 0.16 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 9 | 0.17 | 0.04 | 0.16 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 9 | 0.17 | 0.01 | 0.16 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 9 | 0.15 | 0.02 | 0.15 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 9 | 0.15 | 0.02 | 0.15 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 9 | 0.14 | 0.01 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 9 | 0.14 | 0.01 | 0.14 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 9 | 0.13 | 0.01 | 0.13 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 9 | 0.13 | 0.01 | 0.13 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 9 | 0.12 | 0.02 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 9 | 0.12 | 0.02 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 9 | 0.11 | 0.0 | 0.11 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 8 | 0.2 | 0.06 | 0.2 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 8 | 0.2 | 0.06 | 0.2 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 8 | 0.2 | 0.06 | 0.2 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 8 | 0.2 | 0.06 | 0.2 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 8 | 0.2 | 0.06 | 0.2 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 8 | 0.2 | 0.06 | 0.2 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 8 | 0.19 | 0.04 | 0.18 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 8 | 0.19 | 0.04 | 0.18 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 8 | 0.19 | 0.04 | 0.18 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 8 | 0.17 | 0.05 | 0.18 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 8 | 0.17 | 0.03 | 0.16 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 8 | 0.17 | 0.03 | 0.16 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 8 | 0.15 | 0.02 | 0.15 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 8 | 0.14 | 0.04 | 0.13 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 8 | 0.14 | 0.04 | 0.13 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 8 | 0.14 | 0.04 | 0.13 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 8 | 0.14 | 0.02 | 0.14 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 8 | 0.14 | 0.02 | 0.14 |
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 8 | 0.14 | 0.02 | 0.13 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 8 | 0.14 | 0.02 | 0.13 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 8 | 0.14 | 0.02 | 0.13 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 8 | 0.14 | 0.01 | 0.13 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 8 | 0.13 | 0.01 | 0.14 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 8 | 0.13 | 0.01 | 0.14 |
| (1,221) | 1:A:13:ARG:HH12 | 1:A:85:SER:H | 7 | 0.17 | 0.05 | 0.13 |
| (1,1340) | 1:A:7:ILE:HB | 1:A:75:ASN:HB3 | 7 | 0.15 | 0.03 | 0.16 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE1 | 7 | 0.15 | 0.01 | 0.14 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE2 | 7 | 0.15 | 0.01 | 0.14 |
| (1,633) | 1:A:37:TYR:HA | 1:A:40:ARG:HB2 | 7 | 0.14 | 0.03 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG21 | 7 | 0.14 | 0.03 | 0.14 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG22 | 7 | 0.14 | 0.03 | 0.14 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG23 | 7 | 0.14 | 0.03 | 0.14 |
| (1,713) | 1:A:10:LEU:HD21 | 1:A:35:GLU:HA | 7 | 0.14 | 0.03 | 0.14 |
| (1,713) | 1:A:10:LEU:HD22 | 1:A:35:GLU:HA | 7 | 0.14 | 0.03 | 0.14 |
| (1,713) | 1:A:10:LEU:HD23 | 1:A:35:GLU:HA | 7 | 0.14 | 0.03 | 0.14 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB1 | 7 | 0.14 | 0.03 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB2 | 7 | 0.14 | 0.03 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB3 | 7 | 0.14 | 0.03 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB1 | 7 | 0.14 | 0.03 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB2 | 7 | 0.14 | 0.03 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB3 | 7 | 0.14 | 0.03 | 0.13 |
| (1,682) | 1:A:47:ARG:HG3 | 1:A:48:HIS:H | 7 | 0.13 | 0.02 | 0.13 |
| (1,998) | 1:A:49:PHE:HB2 | 1:A:67:LEU:H | 7 | 0.13 | 0.02 | 0.13 |
| (1,1383) | 1:A:103:PRO:HA | 1:A:106:ASN:HB2 | 7 | 0.12 | 0.01 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD11 | 7 | 0.12 | 0.01 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD12 | 7 | 0.12 | 0.01 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD13 | 7 | 0.12 | 0.01 | 0.12 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD21 | 6 | 0.2 | 0.04 | 0.2 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD22 | 6 | 0.2 | 0.04 | 0.2 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD23 | 6 | 0.2 | 0.04 | 0.2 |
| (1,1134) | 1:A:33:TYR:HD1 | 1:A:82:LYS:HA | 6 | 0.2 | 0.04 | 0.2 |
| (1,1134) | 1:A:33:TYR:HD2 | 1:A:82:LYS:HA | 6 | 0.2 | 0.04 | 0.2 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD11 | 6 | 0.16 | 0.05 | 0.15 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD12 | 6 | 0.16 | 0.05 | 0.15 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD13 | 6 | 0.16 | 0.05 | 0.15 |
| (1,442) | 1:A:14:LEU:HB2 | 1:A:30:GLN:H | 6 | 0.16 | 0.03 | 0.16 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD1 | 6 | 0.16 | 0.02 | 0.16 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD2 | 6 | 0.16 | 0.02 | 0.16 |
| (1,1399) | 1:A:70:GLU:HA | 1:A:72:GLU:HG3 | 6 | 0.15 | 0.03 | 0.15 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD11 | 6 | 0.15 | 0.02 | 0.16 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD12 | 6 | 0.15 | 0.02 | 0.16 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD13 | 6 | 0.15 | 0.02 | 0.16 |
| (1,180) | 1:A:54:PHE:H | 1:A:55:SER:H | 6 | 0.14 | 0.02 | 0.14 |
| (1,1765) | 1:A:30:GLN:HE22 | 1:A:31:LYS:HA | 6 | 0.14 | 0.02 | 0.14 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG21 | 6 | 0.13 | 0.02 | 0.12 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG22 | 6 | 0.13 | 0.02 | 0.12 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG23 | 6 | 0.13 | 0.02 | 0.12 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE1 | 6 | 0.13 | 0.02 | 0.12 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE2 | 6 | 0.13 | 0.02 | 0.12 |
| (1,620) | 1:A:103:PRO:HB3 | 1:A:104:GLN:H | 6 | 0.13 | 0.02 | 0.12 |
| (1,1053) | 1:A:81:VAL:HG21 | 1:A:87:LEU:H | 6 | 0.13 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1053) | 1:A:81:VAL:HG22 | 1:A:87:LEU:H | 6 | 0.13 | 0.01 | 0.12 |
| (1,1053) | 1:A:81:VAL:HG23 | 1:A:87:LEU:H | 6 | 0.13 | 0.01 | 0.12 |
| (1,1116) | 1:A:5:SER:HA | 1:A:45:ASN:HD22 | 6 | 0.13 | 0.01 | 0.13 |
| (1,1507) | 1:A:96:PHE:HD1 | 1:A:101:LEU:HG | 6 | 0.13 | 0.02 | 0.12 |
| (1,1507) | 1:A:96:PHE:HD2 | 1:A:101:LEU:HG | 6 | 0.13 | 0.02 | 0.12 |
| (1,168) | 1:A:103:PRO:HD3 | 1:A:104:GLN:H | 6 | 0.12 | 0.01 | 0.13 |
| (1,176) | 1:A:66:SER:H | 1:A:67:LEU:HB2 | 6 | 0.12 | 0.01 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB2 | 6 | 0.12 | 0.0 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB3 | 6 | 0.12 | 0.0 | 0.12 |
| (1,406) | 1:A:41:ASN:HA | 1:A:42:GLY:H | 6 | 0.12 | 0.0 | 0.12 |
| (1,1870) | 1:A:44:GLU:HA | 1:A:44:GLU:HG2 | 6 | 0.11 | 0.0 | 0.11 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG21 | 5 | 0.17 | 0.03 | 0.17 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG22 | 5 | 0.17 | 0.03 | 0.17 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG23 | 5 | 0.17 | 0.03 | 0.17 |
| (1,1) | 1:A:14:LEU:H | 1:A:15:SER:H | 5 | 0.16 | 0.02 | 0.16 |
| (1,572) | 1:A:104:GLN:HA | 1:A:104:GLN:HG3 | 5 | 0.16 | 0.03 | 0.17 |
| (1,716) | 1:A:71:VAL:HG11 | 1:A:105:LYS:HG2 | 5 | 0.15 | 0.04 | 0.15 |
| (1,716) | 1:A:71:VAL:HG12 | 1:A:105:LYS:HG2 | 5 | 0.15 | 0.04 | 0.15 |
| (1,716) | 1:A:71:VAL:HG13 | 1:A:105:LYS:HG2 | 5 | 0.15 | 0.04 | 0.15 |
| (1,347) | 1:A:116:ILE:HG21 | 1:A:118:SER:HA | 5 | 0.15 | 0.02 | 0.16 |
| (1,347) | 1:A:116:ILE:HG22 | 1:A:118:SER:HA | 5 | 0.15 | 0.02 | 0.16 |
| (1,347) | 1:A:116:ILE:HG23 | 1:A:118:SER:HA | 5 | 0.15 | 0.02 | 0.16 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD1 | 5 | 0.14 | 0.01 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD2 | 5 | 0.14 | 0.01 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD1 | 5 | 0.14 | 0.01 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD2 | 5 | 0.14 | 0.01 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD1 | 5 | 0.14 | 0.01 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD2 | 5 | 0.14 | 0.01 | 0.15 |
| (1,1348) | 1:A:31:LYS:HB3 | 1:A:48:HIS:HB3 | 5 | 0.14 | 0.02 | 0.14 |
| (1,1872) | 1:A:91:TYR:HD1 | 1:A:94:VAL:HB | 5 | 0.14 | 0.02 | 0.13 |
| (1,1872) | 1:A:91:TYR:HD2 | 1:A:94:VAL:HB | 5 | 0.14 | 0.02 | 0.13 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE1 | 5 | 0.14 | 0.02 | 0.14 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE2 | 5 | 0.14 | 0.02 | 0.14 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD11 | 5 | 0.14 | 0.02 | 0.14 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD12 | 5 | 0.14 | 0.02 | 0.14 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD13 | 5 | 0.14 | 0.02 | 0.14 |
| (1,58) | 1:A:82:LYS:H | 1:A:82:LYS:HD2 | 5 | 0.14 | 0.02 | 0.14 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG11 | 5 | 0.14 | 0.02 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG12 | 5 | 0.14 | 0.02 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG13 | 5 | 0.14 | 0.02 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG21 | 5 | 0.14 | 0.02 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG22 | 5 | 0.14 | 0.02 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG23 | 5 | 0.14 | 0.02 | 0.13 |
| (1,651) | 1:A:46:ILE:HG12 | 1:A:47:ARG:H | 5 | 0.13 | 0.01 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD1 | 5 | 0.13 | 0.02 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD2 | 5 | 0.13 | 0.02 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD1 | 5 | 0.13 | 0.02 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD2 | 5 | 0.13 | 0.02 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD1 | 5 | 0.13 | 0.02 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD2 | 5 | 0.13 | 0.02 | 0.13 |
| (1,1901) | 1:A:14:LEU:HD11 | 1:A:18:ASP:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD12 | 1:A:18:ASP:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD13 | 1:A:18:ASP:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD21 | 1:A:18:ASP:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD22 | 1:A:18:ASP:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD23 | 1:A:18:ASP:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,533) | 1:A:38:ALA:HA | 1:A:43:PHE:HB3 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG21 | 5 | 0.11 | 0.0 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG22 | 5 | 0.11 | 0.0 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG23 | 5 | 0.11 | 0.0 | 0.11 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG21 | 4 | 0.18 | 0.03 | 0.18 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG22 | 4 | 0.18 | 0.03 | 0.18 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG23 | 4 | 0.18 | 0.03 | 0.18 |
| (1,1460) | 1:A:6:ARG:HG2 | 1:A:75:ASN:HA | 4 | 0.18 | 0.01 | 0.18 |
| (1,1785) | 1:A:50:THR:HA | 1:A:54:PHE:HZ | 4 | 0.16 | 0.04 | 0.15 |
| (1,1423) | 1:A:13:ARG:HB3 | 1:A:13:ARG:HH12 | 4 | 0.16 | 0.04 | 0.16 |
| (1,1070) | 1:A:104:GLN:H | 1:A:104:GLN:HB2 | 4 | 0.16 | 0.03 | 0.16 |
| (1,293) | 1:A:12:GLU:H | 1:A:50:THR:HA | 4 | 0.15 | 0.02 | 0.16 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE2 | 4 | 0.14 | 0.03 | 0.12 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE3 | 4 | 0.14 | 0.03 | 0.12 |
| (1,1414) | 1:A:44:GLU:H | 1:A:44:GLU:HG3 | 4 | 0.14 | 0.02 | 0.13 |
| (1,227) | 1:A:27:ILE:HD11 | 1:A:53:GLY:H | 4 | 0.13 | 0.01 | 0.13 |
| (1,227) | 1:A:27:ILE:HD12 | 1:A:53:GLY:H | 4 | 0.13 | 0.01 | 0.13 |
| (1,227) | 1:A:27:ILE:HD13 | 1:A:53:GLY:H | 4 | 0.13 | 0.01 | 0.13 |
| (1,488) | 1:A:18:ASP:HB2 | 1:A:19:ASP:H | 4 | 0.12 | 0.01 | 0.12 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG21 | 4 | 0.12 | 0.02 | 0.12 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG22 | 4 | 0.12 | 0.02 | 0.12 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG23 | 4 | 0.12 | 0.02 | 0.12 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG21 | 4 | 0.12 | 0.02 | 0.12 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG22 | 4 | 0.12 | 0.02 | 0.12 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG23 | 4 | 0.12 | 0.02 | 0.12 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG21 | 4 | 0.12 | 0.02 | 0.12 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG22 | 4 | 0.12 | 0.02 | 0.12 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG23 | 4 | 0.12 | 0.02 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1003) | 1:A:75:ASN:H | 1:A:75:ASN:HB3 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD1 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD2 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1011) | 1:A:32:LYS:H | 1:A:48:HIS:HE1 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1323) | 1:A:71:VAL:HA | 1:A:105:LYS:HG2 | 4 | 0.12 | 0.01 | 0.12 |
| (1,969) | 1:A:19:ASP:H | 1:A:19:ASP:HA | 4 | 0.12 | 0.0 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD11 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD12 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD13 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1440) | 1:A:6:ARG:HG3 | 1:A:75:ASN:HA | 4 | 0.12 | 0.01 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG11 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG12 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG13 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG21 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG22 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG23 | 4 | 0.11 | 0.0 | 0.11 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG21 | 3 | 0.2 | 0.0 | 0.2 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG22 | 3 | 0.2 | 0.0 | 0.2 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG23 | 3 | 0.2 | 0.0 | 0.2 |
| (1,250) | 1:A:13:ARG:HH11 | 1:A:86:ARG:HG2 | 3 | 0.15 | 0.06 | 0.11 |
| (1,1214) | 1:A:58:ASN:HA | 1:A:59:PHE:HD1 | 3 | 0.15 | 0.04 | 0.12 |
| (1,1214) | 1:A:58:ASN:HA | 1:A:59:PHE:HD2 | 3 | 0.15 | 0.04 | 0.12 |
| (1,1194) | 1:A:61:ARG:HG2 | 1:A:64:PHE:HE1 | 3 | 0.15 | 0.02 | 0.15 |
| (1,1194) | 1:A:61:ARG:HG2 | 1:A:64:PHE:HE2 | 3 | 0.15 | 0.02 | 0.15 |
| (1,1786) | 1:A:54:PHE:HZ | 1:A:62:PRO:HG3 | 3 | 0.14 | 0.02 | 0.16 |
| (1,205) | 1:A:26:SER:H | 1:A:30:GLN:HE22 | 3 | 0.14 | 0.02 | 0.13 |
| (1,563) | 1:A:99:GLU:HA | 1:A:99:GLU:HG2 | 3 | 0.14 | 0.02 | 0.13 |
| (1,1869) | 1:A:57:VAL:HB | 1:A:58:ASN:HD22 | 3 | 0.14 | 0.02 | 0.13 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD11 | 3 | 0.13 | 0.02 | 0.14 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD12 | 3 | 0.13 | 0.02 | 0.14 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD13 | 3 | 0.13 | 0.02 | 0.14 |
| (1,1877) | 1:A:12:GLU:HB2 | 1:A:50:THR:HA | 3 | 0.13 | 0.01 | 0.14 |
| (1,1877) | 1:A:12:GLU:HB3 | 1:A:50:THR:HA | 3 | 0.13 | 0.01 | 0.14 |
| (1,1068) | 1:A:13:ARG:H | 1:A:86:ARG:HG3 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD11 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD12 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD13 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD11 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD12 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD13 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1807) | 1:A:23:GLU:HA | 1:A:23:GLU:HG2 | 3 | 0.13 | 0.02 | 0.12 |
| (1,1807) | 1:A:23:GLU:HA | 1:A:23:GLU:HG3 | 3 | 0.13 | 0.02 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1390) | 1:A:23:GLU:HA | 1:A:29:ASN:HB2 | 3 | 0.13 | 0.01 | 0.12 |
| (1,549) | 1:A:7:ILE:HA | 1:A:45:ASN:HB2 | 3 | 0.12 | 0.0 | 0.12 |
| (1,549) | 1:A:7:ILE:HA | 1:A:45:ASN:HB3 | 3 | 0.12 | 0.0 | 0.12 |
| (1,733) | 1:A:14:LEU:HD11 | 1:A:30:GLN:HE21 | 3 | 0.12 | 0.0 | 0.12 |
| (1,733) | 1:A:14:LEU:HD12 | 1:A:30:GLN:HE21 | 3 | 0.12 | 0.0 | 0.12 |
| (1,733) | 1:A:14:LEU:HD13 | 1:A:30:GLN:HE21 | 3 | 0.12 | 0.0 | 0.12 |
| (1,733) | 1:A:14:LEU:HD21 | 1:A:30:GLN:HE21 | 3 | 0.12 | 0.0 | 0.12 |
| (1,733) | 1:A:14:LEU:HD22 | 1:A:30:GLN:HE21 | 3 | 0.12 | 0.0 | 0.12 |
| (1,733) | 1:A:14:LEU:HD23 | 1:A:30:GLN:HE21 | 3 | 0.12 | 0.0 | 0.12 |
| (1,1103) | 1:A:41:ASN:H | 1:A:41:ASN:HB3 | 3 | 0.12 | 0.0 | 0.12 |
| (1,1300) | 1:A:78:THR:HG21 | 1:A:107:VAL:HA | 3 | 0.12 | 0.0 | 0.12 |
| (1,1300) | 1:A:78:THR:HG22 | 1:A:107:VAL:HA | 3 | 0.12 | 0.0 | 0.12 |
| (1,1300) | 1:A:78:THR:HG23 | 1:A:107:VAL:HA | 3 | 0.12 | 0.0 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD11 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD12 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD13 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD21 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD22 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD23 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD21 | 3 | 0.12 | 0.01 | 0.13 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD22 | 3 | 0.12 | 0.01 | 0.13 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD23 | 3 | 0.12 | 0.01 | 0.13 |
| (1,1789) | 1:A:78:THR:HA | 1:A:108:ARG:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,1928) | 1:A:107:VAL:HG21 | 1:A:109:PHE:HB3 | 3 | 0.12 | 0.01 | 0.13 |
| (1,1928) | 1:A:107:VAL:HG22 | 1:A:109:PHE:HB3 | 3 | 0.12 | 0.01 | 0.13 |
| (1,1928) | 1:A:107:VAL:HG23 | 1:A:109:PHE:HB3 | 3 | 0.12 | 0.01 | 0.13 |
| (1,438) | 1:A:14:LEU:HB3 | 1:A:30:GLN:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,1109) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HE1 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1109) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HE2 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1853) | 1:A:47:ARG:HA | 1:A:47:ARG:HD2 | 3 | 0.12 | 0.01 | 0.12 |
| (1,1853) | 1:A:47:ARG:HA | 1:A:47:ARG:HD3 | 3 | 0.12 | 0.01 | 0.12 |
| (1,559) | 1:A:44:GLU:HG3 | 1:A:45:ASN:HA | 3 | 0.12 | 0.01 | 0.11 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD11 | 3 | 0.12 | 0.0 | 0.12 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD12 | 3 | 0.12 | 0.0 | 0.12 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD13 | 3 | 0.12 | 0.0 | 0.12 |
| (1,1837) | 1:A:28:THR:HA | 1:A:31:LYS:HD2 | 3 | 0.12 | 0.01 | 0.11 |
| (1,1470) | 1:A:74:GLY:HA3 | 1:A:105:LYS:HG2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG21 | 1:A:102:PHE:HD1 | 3 | 0.11 | 0.0 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG21 | 1:A:102:PHE:HD2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG22 | 1:A:102:PHE:HD1 | 3 | 0.11 | 0.0 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG22 | 1:A:102:PHE:HD2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG23 | 1:A:102:PHE:HD1 | 3 | 0.11 | 0.0 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1620) | 1:A:71:VAL:HG23 | 1:A:102:PHE:HD2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD11 | 2 | 0.24 | 0.03 | 0.24 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD12 | 2 | 0.24 | 0.03 | 0.24 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD13 | 2 | 0.24 | 0.03 | 0.24 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD11 | 2 | 0.24 | 0.03 | 0.24 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD12 | 2 | 0.24 | 0.03 | 0.24 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD13 | 2 | 0.24 | 0.03 | 0.24 |
| (1,695) | 1:A:14:LEU:HG | 1:A:26:SER:HA | 2 | 0.21 | 0.03 | 0.21 |
| (1,121) | 1:A:18:ASP:H | 1:A:20:LEU:HG | 2 | 0.19 | 0.05 | 0.19 |
| (1,997) | 1:A:64:PHE:HD1 | 1:A:67:LEU:H | 2 | 0.17 | 0.01 | 0.17 |
| (1,997) | 1:A:64:PHE:HD2 | 1:A:67:LEU:H | 2 | 0.17 | 0.01 | 0.17 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD21 | 2 | 0.15 | 0.01 | 0.15 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD22 | 2 | 0.15 | 0.01 | 0.15 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD23 | 2 | 0.15 | 0.01 | 0.15 |
| (1,1253) | 1:A:83:ASP:HA | 1:A:111:ALA:HA | 2 | 0.15 | 0.02 | 0.15 |
| (1,88) | 1:A:119:ASN:H | 1:A:120:ASN:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,1740) | 1:A:31:LYS:HA | 1:A:48:HIS:HE1 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1792) | 1:A:13:ARG:HA | 1:A:54:PHE:HD1 | 2 | 0.15 | 0.02 | 0.15 |
| (1,1792) | 1:A:13:ARG:HA | 1:A:54:PHE:HD2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,1534) | 1:A:57:VAL:HG11 | 1:A:58:ASN:HD22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,1534) | 1:A:57:VAL:HG12 | 1:A:58:ASN:HD22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,1534) | 1:A:57:VAL:HG13 | 1:A:58:ASN:HD22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,1534) | 1:A:57:VAL:HG21 | 1:A:58:ASN:HD22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,1534) | 1:A:57:VAL:HG22 | 1:A:58:ASN:HD22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,1534) | 1:A:57:VAL:HG23 | 1:A:58:ASN:HD22 | 2 | 0.14 | 0.03 | 0.14 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD11 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD12 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD13 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD11 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD12 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD13 | 2 | 0.14 | 0.02 | 0.14 |
| (1,665) | 1:A:61:ARG:HA | 1:A:62:PRO:HG3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1054) | 1:A:106:ASN:HB2 | 1:A:106:ASN:HD22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1589) | 1:A:37:TYR:HD1 | 1:A:110:LEU:HG | 2 | 0.14 | 0.01 | 0.14 |
| (1,1589) | 1:A:37:TYR:HD2 | 1:A:110:LEU:HG | 2 | 0.14 | 0.01 | 0.14 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG11 | 2 | 0.13 | 0.02 | 0.13 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG12 | 2 | 0.13 | 0.02 | 0.13 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG13 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1008) | 1:A:112:ILE:H | 1:A:112:ILE:HG12 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1201) | 1:A:59:PHE:HB3 | 1:A:64:PHE:HD1 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1201) | 1:A:59:PHE:HB3 | 1:A:64:PHE:HD2 | 2 | 0.13 | 0.02 | 0.13 |
| (1,256) | 1:A:83:ASP:H | 1:A:86:ARG:HG3 | 2 | 0.12 | 0.02 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,419) | 1:A:60:ASN:HA | 1:A:65:GLN:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,419) | 1:A:60:ASN:HA | 1:A:65:GLN:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,569) | 1:A:27:ILE:HB | 1:A:30:GLN:HE22 | 2 | 0.12 | 0.02 | 0.12 |
| (1,982) | 1:A:43:PHE:H | 1:A:43:PHE:HD1 | 2 | 0.12 | 0.01 | 0.12 |
| (1,982) | 1:A:43:PHE:H | 1:A:43:PHE:HD2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1222) | 1:A:93:GLN:HA | 1:A:96:PHE:HD1 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1222) | 1:A:93:GLN:HA | 1:A:96:PHE:HD2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1823) | 1:A:32:LYS:HA | 1:A:32:LYS:HG2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1830) | 1:A:72:GLU:HA | 1:A:72:GLU:HG2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,222) | 1:A:83:ASP:HA | 1:A:85:SER:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,229) | 1:A:39:ARG:HG2 | 1:A:41:ASN:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,303) | 1:A:10:LEU:H | 1:A:46:ILE:HA | 2 | 0.12 | 0.0 | 0.12 |
| (1,545) | 1:A:35:GLU:H | 1:A:35:GLU:HG3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD11 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD12 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD13 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD11 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD12 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD13 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1432) | 1:A:34:LEU:H | 1:A:34:LEU:HB3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD11 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD13 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD21 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD22 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD23 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD21 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD22 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD23 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD21 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD22 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD23 | 2 | 0.12 | 0.01 | 0.12 |
| (1,666) | 1:A:81:VAL:HG21 | 1:A:87:LEU:HG | 2 | 0.12 | 0.0 | 0.12 |
| (1,666) | 1:A:81:VAL:HG22 | 1:A:87:LEU:HG | 2 | 0.12 | 0.0 | 0.12 |
| (1,666) | 1:A:81:VAL:HG23 | 1:A:87:LEU:HG | 2 | 0.12 | 0.0 | 0.12 |
| (1,54) | 1:A:119:ASN:HA | 1:A:120:ASN:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,110) | 1:A:19:ASP:HA | 1:A:20:LEU:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,1334) | 1:A:111:ALA:H | 1:A:112:ILE:HA | 2 | 0.11 | 0.0 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB1 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1563) | 1:A:68:ILE:HG21 | 1:A:72:GLU:HG3 | 2 | 0.11 | 0.0 | 0.11 |

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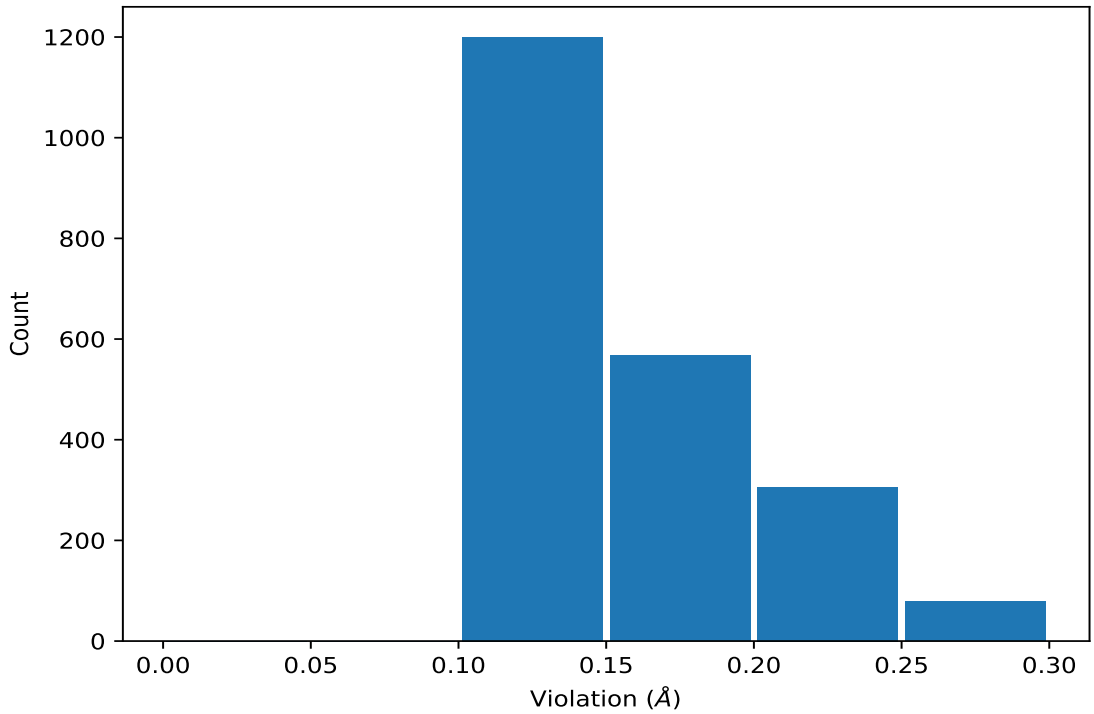
| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1563) | 1:A:68:ILE:HG22 | 1:A:72:GLU:HG3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1563) | 1:A:68:ILE:HG23 | 1:A:72:GLU:HG3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD11 | 1:A:93:GLN:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD11 | 1:A:93:GLN:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD12 | 1:A:93:GLN:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD12 | 1:A:93:GLN:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD13 | 1:A:93:GLN:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD13 | 1:A:93:GLN:HB3 | 2 | 0.11 | 0.0 | 0.11 |

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

## 9.5 All violated distance restraints (i)

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

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




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

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

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 7 | 0.3 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 7 | 0.3 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 7 | 0.3 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 7 | 0.3 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 7 | 0.3 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 7 | 0.3 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 3 | 0.29 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 3 | 0.29 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 3 | 0.29 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 3 | 0.29 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 3 | 0.29 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 3 | 0.29 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 3 | 0.29 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 3 | 0.29 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 3 | 0.29 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 6 | 0.29 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 7 | 0.29 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 8 | 0.28 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 10 | 0.28 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 7 | 0.27 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 6 | 0.27 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 6 | 0.27 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 6 | 0.27 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 6 | 0.27 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 6 | 0.27 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 6 | 0.27 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 6 | 0.27 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 6 | 0.27 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 6 | 0.27 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 9 | 0.27 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 9 | 0.27 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 9 | 0.27 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 7 | 0.27 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD11 | 1 | 0.27 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD12 | 1 | 0.27 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD13 | 1 | 0.27 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD11 | 1 | 0.27 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD12 | 1 | 0.27 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD13 | 1 | 0.27 |
| (1,1134) | 1:A:33:TYR:HD1 | 1:A:82:LYS:HA | 6 | 0.27 |
| (1,1134) | 1:A:33:TYR:HD2 | 1:A:82:LYS:HA | 6 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 4 | 0.27 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 1 | 0.26 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 9 | 0.26 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 2 | 0.26 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 2 | 0.26 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 2 | 0.26 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 2 | 0.26 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 2 | 0.26 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 2 | 0.26 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 2 | 0.26 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 2 | 0.26 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 2 | 0.26 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD21 | 10 | 0.26 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD22 | 10 | 0.26 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD23 | 10 | 0.26 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 6 | 0.26 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 2 | 0.26 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 10 | 0.26 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD11 | 8 | 0.26 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD12 | 8 | 0.26 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD13 | 8 | 0.26 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 8 | 0.26 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 6 | 0.25 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD21 | 2 | 0.25 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD22 | 2 | 0.25 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD23 | 2 | 0.25 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 7 | 0.25 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 6 | 0.25 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 8 | 0.25 |
| (1,221) | 1:A:13:ARG:HH12 | 1:A:85:SER:H | 4 | 0.25 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 10 | 0.25 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 10 | 0.25 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 1 | 0.25 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 1 | 0.25 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 1 | 0.25 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 1 | 0.25 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 1 | 0.25 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 1 | 0.25 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 2 | 0.24 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 2 | 0.24 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 2 | 0.24 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 2 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 2 | 0.24 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 2 | 0.24 |
| (1,695) | 1:A:14:LEU:HG | 1:A:26:SER:HA | 5 | 0.24 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 8 | 0.24 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 8 | 0.24 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 8 | 0.24 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 8 | 0.24 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 8 | 0.24 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 8 | 0.24 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 8 | 0.24 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 8 | 0.24 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 8 | 0.24 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 9 | 0.24 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 1 | 0.24 |
| (1,250) | 1:A:13:ARG:HH11 | 1:A:86:ARG:HG2 | 5 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 4 | 0.24 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 4 | 0.24 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 2 | 0.24 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 2 | 0.24 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 7 | 0.24 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 7 | 0.24 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 7 | 0.24 |
| (1,121) | 1:A:18:ASP:H | 1:A:20:LEU:HG | 5 | 0.24 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 9 | 0.24 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 2 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 1 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 1 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 1 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 1 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 1 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 1 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 1 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 1 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 1 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 7 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 9 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 9 | 0.23 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 9 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 9 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 9 | 0.23 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 9 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 9 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 9 | 0.23 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 9 | 0.23 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG21 | 7 | 0.23 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG22 | 7 | 0.23 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG23 | 7 | 0.23 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 2 | 0.23 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 2 | 0.23 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 2 | 0.23 |
| (1,160) | 1:A:45:ASN:HA | 1:A:46:ILE:H | 5 | 0.23 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 8 | 0.23 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 8 | 0.23 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 7 | 0.23 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 7 | 0.23 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 8 | 0.23 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 8 | 0.23 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 10 | 0.23 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 10 | 0.23 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 3 | 0.23 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 10 | 0.23 |
| (1,716) | 1:A:71:VAL:HG11 | 1:A:105:LYS:HG2 | 6 | 0.22 |
| (1,716) | 1:A:71:VAL:HG12 | 1:A:105:LYS:HG2 | 6 | 0.22 |
| (1,716) | 1:A:71:VAL:HG13 | 1:A:105:LYS:HG2 | 6 | 0.22 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 4 | 0.22 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 4 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 4 | 0.22 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 4 | 0.22 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 4 | 0.22 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 4 | 0.22 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 4 | 0.22 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 4 | 0.22 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 4 | 0.22 |
| (1,633) | 1:A:37:TYR:HA | 1:A:40:ARG:HB2 | 8 | 0.22 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 4 | 0.22 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 4 | 0.22 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 4 | 0.22 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 9 | 0.22 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 10 | 0.22 |
| (1,442) | 1:A:14:LEU:HB2 | 1:A:30:GLN:H | 1 | 0.22 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 9 | 0.22 |
| (1,221) | 1:A:13:ARG:HH12 | 1:A:85:SER:H | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 6 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 8 | 0.22 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 8 | 0.22 |
| (1,1785) | 1:A:50:THR:HA | 1:A:54:PHE:HZ | 4 | 0.22 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 9 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 9 | 0.22 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 9 | 0.22 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 9 | 0.22 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 9 | 0.22 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 9 | 0.22 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 1 | 0.22 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 1 | 0.22 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 1 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 3 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 3 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 3 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 3 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 3 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 3 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 9 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 9 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 9 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 9 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 9 | 0.22 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 9 | 0.22 |
| (1,1478) | 1:A:27:ILE:HG12 | 1:A:51:ASP:H | 2 | 0.22 |
| (1,1478) | 1:A:27:ILE:HG13 | 1:A:51:ASP:H | 2 | 0.22 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 9 | 0.22 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 9 | 0.22 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 10 | 0.22 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 10 | 0.22 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 9 | 0.22 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 9 | 0.22 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 1 | 0.22 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 5 | 0.22 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 6 | 0.22 |
| (1,1134) | 1:A:33:TYR:HD1 | 1:A:82:LYS:HA | 9 | 0.22 |
| (1,1134) | 1:A:33:TYR:HD2 | 1:A:82:LYS:HA | 9 | 0.22 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 4 | 0.22 |
| (1,1127) | 1:A:48:HIS:HB2 | 1:A:48:HIS:HD2 | 2 | 0.22 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 1 | 0.22 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 10 | 0.21 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 10 | 0.21 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 10 | 0.21 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 10 | 0.21 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 10 | 0.21 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 10 | 0.21 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 10 | 0.21 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 10 | 0.21 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD21 | 7 | 0.21 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD22 | 7 | 0.21 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD23 | 7 | 0.21 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 4 | 0.21 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 5 | 0.21 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 5 | 0.21 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 6 | 0.21 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 3 | 0.21 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 3 | 0.21 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 3 | 0.21 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 7 | 0.21 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 7 | 0.21 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 7 | 0.21 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 7 | 0.21 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 7 | 0.21 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 7 | 0.21 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD11 | 3 | 0.21 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD12 | 3 | 0.21 |
| (1,1516) | 1:A:47:ARG:HD2 | 1:A:7:ILE:HD13 | 3 | 0.21 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD11 | 3 | 0.21 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD12 | 3 | 0.21 |
| (1,1516) | 1:A:47:ARG:HD3 | 1:A:7:ILE:HD13 | 3 | 0.21 |
| (1,1423) | 1:A:13:ARG:HB3 | 1:A:13:ARG:HH12 | 3 | 0.21 |
| (1,1371) | 1:A:119:ASN:HB3 | 1:A:120:ASN:HA | 2 | 0.21 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 3 | 0.21 |
| (1,1214) | 1:A:58:ASN:HA | 1:A:59:PHE:HD1 | 6 | 0.21 |
| (1,1214) | 1:A:58:ASN:HA | 1:A:59:PHE:HD2 | 6 | 0.21 |
| (1,1134) | 1:A:33:TYR:HD1 | 1:A:82:LYS:HA | 8 | 0.21 |
| (1,1134) | 1:A:33:TYR:HD2 | 1:A:82:LYS:HA | 8 | 0.21 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 7 | 0.21 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 7 | 0.21 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 8 | 0.21 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 8 | 0.21 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 2 | 0.21 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 3 | 0.2 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 5 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 3 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 3 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 3 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 3 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 3 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 7 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 7 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 7 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 7 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 7 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 7 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 9 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 9 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 9 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 9 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 9 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 9 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 10 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 10 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 10 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 10 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 10 | 0.2 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 10 | 0.2 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 8 | 0.2 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 8 | 0.2 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD21 | 1 | 0.2 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD22 | 1 | 0.2 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD23 | 1 | 0.2 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 1 | 0.2 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 1 | 0.2 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 1 | 0.2 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE2 | 6 | 0.2 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE3 | 6 | 0.2 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 3 | 0.2 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG21 | 4 | 0.2 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG22 | 4 | 0.2 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG23 | 4 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 2 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 2 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 9 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 10 | 0.2 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 10 | 0.2 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG21 | 1 | 0.2 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG22 | 1 | 0.2 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG23 | 1 | 0.2 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG21 | 7 | 0.2 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG22 | 7 | 0.2 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG23 | 7 | 0.2 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG21 | 9 | 0.2 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG22 | 9 | 0.2 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG23 | 9 | 0.2 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB1 | 10 | 0.2 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB2 | 10 | 0.2 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB3 | 10 | 0.2 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB1 | 10 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB2 | 10 | 0.2 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB3 | 10 | 0.2 |
| (1,1460) | 1:A:6:ARG:HG2 | 1:A:75:ASN:HA | 4 | 0.2 |
| (1,1399) | 1:A:70:GLU:HA | 1:A:72:GLU:HG3 | 1 | 0.2 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 6 | 0.2 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 6 | 0.2 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 8 | 0.2 |
| (1,1006) | 1:A:81:VAL:HB | 1:A:112:ILE:H | 5 | 0.2 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 4 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 5 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 5 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 5 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 5 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 5 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 5 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 8 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 8 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 8 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 8 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 8 | 0.19 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 8 | 0.19 |
| (1,713) | 1:A:10:LEU:HD21 | 1:A:35:GLU:HA | 8 | 0.19 |
| (1,713) | 1:A:10:LEU:HD22 | 1:A:35:GLU:HA | 8 | 0.19 |
| (1,713) | 1:A:10:LEU:HD23 | 1:A:35:GLU:HA | 8 | 0.19 |
| (1,671) | 1:A:105:LYS:HB3 | 1:A:105:LYS:HD2 | 3 | 0.19 |
| (1,671) | 1:A:105:LYS:HB3 | 1:A:105:LYS:HD3 | 3 | 0.19 |
| (1,572) | 1:A:104:GLN:HA | 1:A:104:GLN:HG3 | 10 | 0.19 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 8 | 0.19 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 8 | 0.19 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 8 | 0.19 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 1 | 0.19 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 4 | 0.19 |
| (1,221) | 1:A:13:ARG:HH12 | 1:A:85:SER:H | 10 | 0.19 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG21 | 8 | 0.19 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG22 | 8 | 0.19 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG23 | 8 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 7 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 7 | 0.19 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 7 | 0.19 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 8 | 0.19 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 8 | 0.19 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 8 | 0.19 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG21 | 1 | 0.19 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG22 | 1 | 0.19 |
| (1,1888) | 1:A:4:THR:HA | 1:A:4:THR:HG23 | 1 | 0.19 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD1 | 9 | 0.19 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD2 | 9 | 0.19 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 1 | 0.19 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 2 | 0.19 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 5 | 0.19 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 7 | 0.19 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 3 | 0.19 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 3 | 0.19 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 5 | 0.19 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 5 | 0.19 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 4 | 0.19 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 4 | 0.19 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 4 | 0.19 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 4 | 0.19 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 4 | 0.19 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 4 | 0.19 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 8 | 0.19 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 8 | 0.19 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 8 | 0.19 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG21 | 4 | 0.19 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG22 | 4 | 0.19 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG23 | 4 | 0.19 |
| (1,1340) | 1:A:7:ILE:HB | 1:A:75:ASN:HB3 | 8 | 0.19 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 9 | 0.19 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 2 | 0.19 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 2 | 0.19 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 6 | 0.19 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 6 | 0.19 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 2 | 0.19 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 2 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 4 | 0.19 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 4 | 0.19 |
| (1,1134) | 1:A:33:TYR:HD1 | 1:A:82:LYS:HA | 4 | 0.19 |
| (1,1134) | 1:A:33:TYR:HD2 | 1:A:82:LYS:HA | 4 | 0.19 |
| (1,1070) | 1:A:104:GLN:H | 1:A:104:GLN:HB2 | 3 | 0.19 |
| (1,997) | 1:A:64:PHE:HD1 | 1:A:67:LEU:H | 9 | 0.18 |
| (1,997) | 1:A:64:PHE:HD2 | 1:A:67:LEU:H | 9 | 0.18 |
| (1,994) | 1:A:46:ILE:H | 1:A:46:ILE:HB | 5 | 0.18 |
| (1,695) | 1:A:14:LEU:HG | 1:A:26:SER:HA | 1 | 0.18 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 1 | 0.18 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 2 | 0.18 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 3 | 0.18 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 8 | 0.18 |
| (1,442) | 1:A:14:LEU:HB2 | 1:A:30:GLN:H | 8 | 0.18 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 5 | 0.18 |
| (1,1872) | 1:A:91:TYR:HD1 | 1:A:94:VAL:HB | 10 | 0.18 |
| (1,1872) | 1:A:91:TYR:HD2 | 1:A:94:VAL:HB | 10 | 0.18 |
| (1,1785) | 1:A:50:THR:HA | 1:A:54:PHE:HZ | 5 | 0.18 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD1 | 8 | 0.18 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD2 | 8 | 0.18 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 4 | 0.18 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 10 | 0.18 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 4 | 0.18 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 4 | 0.18 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 10 | 0.18 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 10 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 5 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 5 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 5 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 5 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 5 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 5 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 6 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 6 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 6 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 6 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 6 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 6 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 10 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 10 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 10 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 10 | 0.18 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 10 | 0.18 |
| (1,1626) | 1:A:64:PHE:HE1 | 1:A:67:LEU:HG | 10 | 0.18 |
| (1,1626) | 1:A:64:PHE:HE2 | 1:A:67:LEU:HG | 10 | 0.18 |
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 7 | 0.18 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 7 | 0.18 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 7 | 0.18 |
| (1,1460) | 1:A:6:ARG:HG2 | 1:A:75:ASN:HA | 5 | 0.18 |
| (1,1414) | 1:A:44:GLU:H | 1:A:44:GLU:HG3 | 6 | 0.18 |
| (1,1399) | 1:A:70:GLU:HA | 1:A:72:GLU:HG3 | 7 | 0.18 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 1 | 0.18 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 5 | 0.18 |
| (1,1340) | 1:A:7:ILE:HB | 1:A:75:ASN:HB3 | 7 | 0.18 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 2 | 0.18 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 7 | 0.18 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 4 | 0.18 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 4 | 0.18 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 9 | 0.18 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 10 | 0.18 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 10 | 0.18 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 10 | 0.18 |
| (1,1164) | 1:A:37:TYR:HA | 1:A:37:TYR:HD1 | 8 | 0.18 |
| (1,1164) | 1:A:37:TYR:HA | 1:A:37:TYR:HD2 | 8 | 0.18 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 10 | 0.18 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 8 | 0.18 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 10 | 0.18 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 2 | 0.18 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 2 | 0.18 |
| (1,1) | 1:A:14:LEU:H | 1:A:15:SER:H | 1 | 0.18 |
| (1,88) | 1:A:119:ASN:H | 1:A:120:ASN:H | 10 | 0.17 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 4 | 0.17 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 4 | 0.17 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 4 | 0.17 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 4 | 0.17 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 4 | 0.17 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 4 | 0.17 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG21 | 5 | 0.17 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG22 | 5 | 0.17 |
| (1,692) | 1:A:79:LEU:HD21 | 1:A:81:VAL:HG23 | 5 | 0.17 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG21 | 5 | 0.17 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG22 | 5 | 0.17 |
| (1,692) | 1:A:79:LEU:HD22 | 1:A:81:VAL:HG23 | 5 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG21 | 5 | 0.17 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG22 | 5 | 0.17 |
| (1,692) | 1:A:79:LEU:HD23 | 1:A:81:VAL:HG23 | 5 | 0.17 |
| (1,682) | 1:A:47:ARG:HG3 | 1:A:48:HIS:H | 7 | 0.17 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE1 | 5 | 0.17 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE2 | 5 | 0.17 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 3 | 0.17 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 3 | 0.17 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 5 | 0.17 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 5 | 0.17 |
| (1,58) | 1:A:82:LYS:H | 1:A:82:LYS:HD2 | 8 | 0.17 |
| (1,572) | 1:A:104:GLN:HA | 1:A:104:GLN:HG3 | 4 | 0.17 |
| (1,572) | 1:A:104:GLN:HA | 1:A:104:GLN:HG3 | 7 | 0.17 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD21 | 3 | 0.17 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD22 | 3 | 0.17 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD23 | 3 | 0.17 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 7 | 0.17 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 4 | 0.17 |
| (1,462) | 1:A:61:ARG:HD2 | 1:A:64:PHE:HE1 | 8 | 0.17 |
| (1,462) | 1:A:61:ARG:HD2 | 1:A:64:PHE:HE2 | 8 | 0.17 |
| (1,462) | 1:A:61:ARG:HD3 | 1:A:64:PHE:HE1 | 8 | 0.17 |
| (1,462) | 1:A:61:ARG:HD3 | 1:A:64:PHE:HE2 | 8 | 0.17 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG11 | 6 | 0.17 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG12 | 6 | 0.17 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG13 | 6 | 0.17 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG21 | 6 | 0.17 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG22 | 6 | 0.17 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG23 | 6 | 0.17 |
| (1,422) | 1:A:58:ASN:HA | 1:A:87:LEU:HA | 8 | 0.17 |
| (1,347) | 1:A:116:ILE:HG21 | 1:A:118:SER:HA | 9 | 0.17 |
| (1,347) | 1:A:116:ILE:HG22 | 1:A:118:SER:HA | 9 | 0.17 |
| (1,347) | 1:A:116:ILE:HG23 | 1:A:118:SER:HA | 9 | 0.17 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 7 | 0.17 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 8 | 0.17 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 9 | 0.17 |
| (1,293) | 1:A:12:GLU:H | 1:A:50:THR:HA | 1 | 0.17 |
| (1,293) | 1:A:12:GLU:H | 1:A:50:THR:HA | 2 | 0.17 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG21 | 9 | 0.17 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG22 | 9 | 0.17 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG23 | 9 | 0.17 |
| (1,205) | 1:A:26:SER:H | 1:A:30:GLN:HE22 | 4 | 0.17 |
| (1,1901) | 1:A:14:LEU:HD11 | 1:A:18:ASP:HB2 | 1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1901) | 1:A:14:LEU:HD12 | 1:A:18:ASP:HB2 | 1 | 0.17 |
| (1,1901) | 1:A:14:LEU:HD13 | 1:A:18:ASP:HB2 | 1 | 0.17 |
| (1,1901) | 1:A:14:LEU:HD21 | 1:A:18:ASP:HB2 | 1 | 0.17 |
| (1,1901) | 1:A:14:LEU:HD22 | 1:A:18:ASP:HB2 | 1 | 0.17 |
| (1,1901) | 1:A:14:LEU:HD23 | 1:A:18:ASP:HB2 | 1 | 0.17 |
| (1,1869) | 1:A:57:VAL:HB | 1:A:58:ASN:HD22 | 8 | 0.17 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD11 | 7 | 0.17 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD12 | 7 | 0.17 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD13 | 7 | 0.17 |
| (1,180) | 1:A:54:PHE:H | 1:A:55:SER:H | 5 | 0.17 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 8 | 0.17 |
| (1,1765) | 1:A:30:GLN:HE22 | 1:A:31:LYS:HA | 1 | 0.17 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 9 | 0.17 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 9 | 0.17 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 3 | 0.17 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 3 | 0.17 |
| (1,1740) | 1:A:31:LYS:HA | 1:A:48:HIS:HE1 | 5 | 0.17 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD11 | 5 | 0.17 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD12 | 5 | 0.17 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD13 | 5 | 0.17 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 3 | 0.17 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 3 | 0.17 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 3 | 0.17 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 3 | 0.17 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 3 | 0.17 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 3 | 0.17 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 6 | 0.17 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 6 | 0.17 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 6 | 0.17 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 6 | 0.17 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 6 | 0.17 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 6 | 0.17 |
| (1,1534) | 1:A:57:VAL:HG11 | 1:A:58:ASN:HD22 | 10 | 0.17 |
| (1,1534) | 1:A:57:VAL:HG12 | 1:A:58:ASN:HD22 | 10 | 0.17 |
| (1,1534) | 1:A:57:VAL:HG13 | 1:A:58:ASN:HD22 | 10 | 0.17 |
| (1,1534) | 1:A:57:VAL:HG21 | 1:A:58:ASN:HD22 | 10 | 0.17 |
| (1,1534) | 1:A:57:VAL:HG22 | 1:A:58:ASN:HD22 | 10 | 0.17 |
| (1,1534) | 1:A:57:VAL:HG23 | 1:A:58:ASN:HD22 | 10 | 0.17 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 10 | 0.17 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 10 | 0.17 |
| (1,1460) | 1:A:6:ARG:HG2 | 1:A:75:ASN:HA | 7 | 0.17 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD11 | 1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD12 | 1 | 0.17 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD13 | 1 | 0.17 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE1 | 9 | 0.17 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE2 | 9 | 0.17 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG21 | 6 | 0.17 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG22 | 6 | 0.17 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG23 | 6 | 0.17 |
| (1,1348) | 1:A:31:LYS:HB3 | 1:A:48:HIS:HB3 | 7 | 0.17 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 3 | 0.17 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 8 | 0.17 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 6 | 0.17 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 1 | 0.17 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 1 | 0.17 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 2 | 0.17 |
| (1,1253) | 1:A:83:ASP:HA | 1:A:111:ALA:HA | 4 | 0.17 |
| (1,1194) | 1:A:61:ARG:HG2 | 1:A:64:PHE:HE1 | 1 | 0.17 |
| (1,1194) | 1:A:61:ARG:HG2 | 1:A:64:PHE:HE2 | 1 | 0.17 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 2 | 0.17 |
| (1,1151) | 1:A:22:GLY:HA2 | 1:A:25:ASN:HD21 | 7 | 0.17 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 2 | 0.17 |
| (1,1070) | 1:A:104:GLN:H | 1:A:104:GLN:HB2 | 8 | 0.17 |
| (1,1) | 1:A:14:LEU:H | 1:A:15:SER:H | 4 | 0.17 |
| (1,998) | 1:A:49:PHE:HB2 | 1:A:67:LEU:H | 6 | 0.16 |
| (1,997) | 1:A:64:PHE:HD1 | 1:A:67:LEU:H | 8 | 0.16 |
| (1,997) | 1:A:64:PHE:HD2 | 1:A:67:LEU:H | 8 | 0.16 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 1 | 0.16 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 10 | 0.16 |
| (1,834) | 1:A:9:ALA:H | 1:A:79:LEU:HB3 | 4 | 0.16 |
| (1,778) | 1:A:73:ALA:HB1 | 1:A:75:ASN:HB3 | 1 | 0.16 |
| (1,778) | 1:A:73:ALA:HB2 | 1:A:75:ASN:HB3 | 1 | 0.16 |
| (1,778) | 1:A:73:ALA:HB3 | 1:A:75:ASN:HB3 | 1 | 0.16 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG11 | 1 | 0.16 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG12 | 1 | 0.16 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG13 | 1 | 0.16 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG21 | 1 | 0.16 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG22 | 1 | 0.16 |
| (1,746) | 1:A:91:TYR:HB2 | 1:A:94:VAL:HG23 | 1 | 0.16 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE1 | 4 | 0.16 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE2 | 4 | 0.16 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 9 | 0.16 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 9 | 0.16 |
| (1,620) | 1:A:103:PRO:HB3 | 1:A:104:GLN:H | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,563) | 1:A:99:GLU:HA | 1:A:99:GLU:HG2 | 6 | 0.16 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD21 | 9 | 0.16 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD22 | 9 | 0.16 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD23 | 9 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 2 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 2 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 2 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 3 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 3 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 3 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 7 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 7 | 0.16 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 7 | 0.16 |
| (1,501) | 1:A:11:TYR:HB3 | 1:A:67:LEU:HB2 | 3 | 0.16 |
| (1,442) | 1:A:14:LEU:HB2 | 1:A:30:GLN:H | 2 | 0.16 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE1 | 10 | 0.16 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE2 | 10 | 0.16 |
| (1,347) | 1:A:116:ILE:HG21 | 1:A:118:SER:HA | 1 | 0.16 |
| (1,347) | 1:A:116:ILE:HG22 | 1:A:118:SER:HA | 1 | 0.16 |
| (1,347) | 1:A:116:ILE:HG23 | 1:A:118:SER:HA | 1 | 0.16 |
| (1,347) | 1:A:116:ILE:HG21 | 1:A:118:SER:HA | 2 | 0.16 |
| (1,347) | 1:A:116:ILE:HG22 | 1:A:118:SER:HA | 2 | 0.16 |
| (1,347) | 1:A:116:ILE:HG23 | 1:A:118:SER:HA | 2 | 0.16 |
| (1,278) | 1:A:26:SER:HB2 | 1:A:27:ILE:HB | 10 | 0.16 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 7 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 3 | 0.16 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 3 | 0.16 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG21 | 6 | 0.16 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG22 | 6 | 0.16 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG23 | 6 | 0.16 |
| (1,1807) | 1:A:23:GLU:HA | 1:A:23:GLU:HG2 | 8 | 0.16 |
| (1,1807) | 1:A:23:GLU:HA | 1:A:23:GLU:HG3 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,180) | 1:A:54:PHE:H | 1:A:55:SER:H | 1 | 0.16 |
| (1,1792) | 1:A:13:ARG:HA | 1:A:54:PHE:HD1 | 5 | 0.16 |
| (1,1792) | 1:A:13:ARG:HA | 1:A:54:PHE:HD2 | 5 | 0.16 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 2 | 0.16 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 2 | 0.16 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 3 | 0.16 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 3 | 0.16 |
| (1,1786) | 1:A:54:PHE:HZ | 1:A:62:PRO:HG3 | 1 | 0.16 |
| (1,1786) | 1:A:54:PHE:HZ | 1:A:62:PRO:HG3 | 6 | 0.16 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD1 | 7 | 0.16 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD2 | 7 | 0.16 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD1 | 10 | 0.16 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD2 | 10 | 0.16 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 3 | 0.16 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD1 | 3 | 0.16 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD2 | 3 | 0.16 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD1 | 3 | 0.16 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD2 | 3 | 0.16 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD1 | 3 | 0.16 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD2 | 3 | 0.16 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD11 | 4 | 0.16 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD12 | 4 | 0.16 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD13 | 4 | 0.16 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD11 | 10 | 0.16 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD12 | 10 | 0.16 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD13 | 10 | 0.16 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 7 | 0.16 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 7 | 0.16 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 7 | 0.16 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 9 | 0.16 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 9 | 0.16 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 9 | 0.16 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD11 | 7 | 0.16 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD12 | 7 | 0.16 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD13 | 7 | 0.16 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD11 | 7 | 0.16 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD12 | 7 | 0.16 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD13 | 7 | 0.16 |
| (1,1568) | 1:A:20:LEU:HD11 | 1:A:25:ASN:HB2 | 3 | 0.16 |
| (1,1568) | 1:A:20:LEU:HD12 | 1:A:25:ASN:HB2 | 3 | 0.16 |
| (1,1568) | 1:A:20:LEU:HD13 | 1:A:25:ASN:HB2 | 3 | 0.16 |
| (1,1568) | 1:A:20:LEU:HD21 | 1:A:25:ASN:HB2 | 3 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1568) | 1:A:20:LEU:HD22 | 1:A:25:ASN:HB2 | 3 | 0.16 |
| (1,1568) | 1:A:20:LEU:HD23 | 1:A:25:ASN:HB2 | 3 | 0.16 |
| (1,1507) | 1:A:96:PHE:HD1 | 1:A:101:LEU:HG | 6 | 0.16 |
| (1,1507) | 1:A:96:PHE:HD2 | 1:A:101:LEU:HG | 6 | 0.16 |
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 6 | 0.16 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 6 | 0.16 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 6 | 0.16 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG21 | 10 | 0.16 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG22 | 10 | 0.16 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG23 | 10 | 0.16 |
| (1,1460) | 1:A:6:ARG:HG2 | 1:A:75:ASN:HA | 8 | 0.16 |
| (1,1423) | 1:A:13:ARG:HB3 | 1:A:13:ARG:HH12 | 4 | 0.16 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 2 | 0.16 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD11 | 7 | 0.16 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD12 | 7 | 0.16 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD13 | 7 | 0.16 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE1 | 10 | 0.16 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE2 | 10 | 0.16 |
| (1,1399) | 1:A:70:GLU:HA | 1:A:72:GLU:HG3 | 5 | 0.16 |
| (1,1340) | 1:A:7:ILE:HB | 1:A:75:ASN:HB3 | 1 | 0.16 |
| (1,1340) | 1:A:7:ILE:HB | 1:A:75:ASN:HB3 | 9 | 0.16 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 4 | 0.16 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 8 | 0.16 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 10 | 0.16 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 7 | 0.16 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 10 | 0.16 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 2 | 0.16 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 2 | 0.16 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 7 | 0.16 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 9 | 0.16 |
| (1,1134) | 1:A:33:TYR:HD1 | 1:A:82:LYS:HA | 7 | 0.16 |
| (1,1134) | 1:A:33:TYR:HD2 | 1:A:82:LYS:HA | 7 | 0.16 |
| (1,1134) | 1:A:33:TYR:HD1 | 1:A:82:LYS:HA | 10 | 0.16 |
| (1,1134) | 1:A:33:TYR:HD2 | 1:A:82:LYS:HA | 10 | 0.16 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 1 | 0.16 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 1 | 0.16 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 9 | 0.16 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 9 | 0.16 |
| (1,1) | 1:A:14:LEU:H | 1:A:15:SER:H | 8 | 0.16 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 2 | 0.15 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 8 | 0.15 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,716) | 1:A:71:VAL:HG11 | 1:A:105:LYS:HG2 | 3 | 0.15 |
| (1,716) | 1:A:71:VAL:HG12 | 1:A:105:LYS:HG2 | 3 | 0.15 |
| (1,716) | 1:A:71:VAL:HG13 | 1:A:105:LYS:HG2 | 3 | 0.15 |
| (1,716) | 1:A:71:VAL:HG11 | 1:A:105:LYS:HG2 | 9 | 0.15 |
| (1,716) | 1:A:71:VAL:HG12 | 1:A:105:LYS:HG2 | 9 | 0.15 |
| (1,716) | 1:A:71:VAL:HG13 | 1:A:105:LYS:HG2 | 9 | 0.15 |
| (1,713) | 1:A:10:LEU:HD21 | 1:A:35:GLU:HA | 3 | 0.15 |
| (1,713) | 1:A:10:LEU:HD22 | 1:A:35:GLU:HA | 3 | 0.15 |
| (1,713) | 1:A:10:LEU:HD23 | 1:A:35:GLU:HA | 3 | 0.15 |
| (1,665) | 1:A:61:ARG:HA | 1:A:62:PRO:HG3 | 6 | 0.15 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 6 | 0.15 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 6 | 0.15 |
| (1,633) | 1:A:37:TYR:HA | 1:A:40:ARG:HB2 | 6 | 0.15 |
| (1,620) | 1:A:103:PRO:HB3 | 1:A:104:GLN:H | 6 | 0.15 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG11 | 3 | 0.15 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG12 | 3 | 0.15 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG13 | 3 | 0.15 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 5 | 0.15 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 5 | 0.15 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 5 | 0.15 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG11 | 9 | 0.15 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG12 | 9 | 0.15 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG13 | 9 | 0.15 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG21 | 9 | 0.15 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG22 | 9 | 0.15 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG23 | 9 | 0.15 |
| (1,442) | 1:A:14:LEU:HB2 | 1:A:30:GLN:H | 10 | 0.15 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 7 | 0.15 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 7 | 0.15 |
| (1,395) | 1:A:44:GLU:HA | 1:A:46:ILE:HG13 | 5 | 0.15 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE1 | 6 | 0.15 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE2 | 6 | 0.15 |
| (1,347) | 1:A:116:ILE:HG21 | 1:A:118:SER:HA | 7 | 0.15 |
| (1,347) | 1:A:116:ILE:HG22 | 1:A:118:SER:HA | 7 | 0.15 |
| (1,347) | 1:A:116:ILE:HG23 | 1:A:118:SER:HA | 7 | 0.15 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 6 | 0.15 |
| (1,293) | 1:A:12:GLU:H | 1:A:50:THR:HA | 8 | 0.15 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 3 | 0.15 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG21 | 2 | 0.15 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG22 | 2 | 0.15 |
| (1,1897) | 1:A:18:ASP:HB2 | 1:A:21:THR:HG23 | 2 | 0.15 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 9 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 9 | 0.15 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 9 | 0.15 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD11 | 9 | 0.15 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD12 | 9 | 0.15 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD13 | 9 | 0.15 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD1 | 1 | 0.15 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD2 | 1 | 0.15 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 9 | 0.15 |
| (1,1765) | 1:A:30:GLN:HE22 | 1:A:31:LYS:HA | 3 | 0.15 |
| (1,1765) | 1:A:30:GLN:HE22 | 1:A:31:LYS:HA | 5 | 0.15 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 4 | 0.15 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 4 | 0.15 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 8 | 0.15 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 8 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD1 | 4 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD2 | 4 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD1 | 4 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD2 | 4 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD1 | 4 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD2 | 4 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD1 | 9 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD2 | 9 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD1 | 9 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD2 | 9 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD1 | 9 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD2 | 9 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD1 | 10 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD2 | 10 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD1 | 10 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD2 | 10 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD1 | 10 | 0.15 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD2 | 10 | 0.15 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD11 | 3 | 0.15 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD12 | 3 | 0.15 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD13 | 3 | 0.15 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 1 | 0.15 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 1 | 0.15 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 1 | 0.15 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 1 | 0.15 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 1 | 0.15 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 1 | 0.15 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 4 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 4 | 0.15 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 4 | 0.15 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 10 | 0.15 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 10 | 0.15 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 10 | 0.15 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD11 | 7 | 0.15 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD12 | 7 | 0.15 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD13 | 7 | 0.15 |
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 10 | 0.15 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 10 | 0.15 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 10 | 0.15 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB1 | 2 | 0.15 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB2 | 2 | 0.15 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB3 | 2 | 0.15 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB1 | 2 | 0.15 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB2 | 2 | 0.15 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB3 | 2 | 0.15 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 1 | 0.15 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 1 | 0.15 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 2 | 0.15 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 9 | 0.15 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG21 | 7 | 0.15 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG22 | 7 | 0.15 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG23 | 7 | 0.15 |
| (1,1423) | 1:A:13:ARG:HB3 | 1:A:13:ARG:HH12 | 9 | 0.15 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 1 | 0.15 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 8 | 0.15 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 7 | 0.15 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 7 | 0.15 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 8 | 0.15 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 8 | 0.15 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE1 | 8 | 0.15 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE2 | 8 | 0.15 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG21 | 8 | 0.15 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG22 | 8 | 0.15 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG23 | 8 | 0.15 |
| (1,1383) | 1:A:103:PRO:HA | 1:A:106:ASN:HB2 | 10 | 0.15 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 6 | 0.15 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 3 | 0.15 |
| (1,1265) | 1:A:74:GLY:HA3 | 1:A:104:GLN:HB2 | 4 | 0.15 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 1 | 0.15 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,124) | 1:A:17:ASP:HB2 | 1:A:18:ASP:H | 2 | 0.15 |
| (1,1201) | 1:A:59:PHE:HB3 | 1:A:64:PHE:HD1 | 10 | 0.15 |
| (1,1201) | 1:A:59:PHE:HB3 | 1:A:64:PHE:HD2 | 10 | 0.15 |
| (1,1194) | 1:A:61:ARG:HG2 | 1:A:64:PHE:HE1 | 10 | 0.15 |
| (1,1194) | 1:A:61:ARG:HG2 | 1:A:64:PHE:HE2 | 10 | 0.15 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 5 | 0.15 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 5 | 0.15 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 7 | 0.15 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 7 | 0.15 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 6 | 0.15 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 3 | 0.15 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 5 | 0.15 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 7 | 0.15 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 9 | 0.15 |
| (1,1116) | 1:A:5:SER:HA | 1:A:45:ASN:HD22 | 5 | 0.15 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 6 | 0.15 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 6 | 0.15 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 10 | 0.15 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 10 | 0.15 |
| (1,1053) | 1:A:81:VAL:HG21 | 1:A:87:LEU:H | 1 | 0.15 |
| (1,1053) | 1:A:81:VAL:HG22 | 1:A:87:LEU:H | 1 | 0.15 |
| (1,1053) | 1:A:81:VAL:HG23 | 1:A:87:LEU:H | 1 | 0.15 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 4 | 0.15 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 5 | 0.15 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 9 | 0.15 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 10 | 0.15 |
| (1,1008) | 1:A:112:ILE:H | 1:A:112:ILE:HG12 | 6 | 0.15 |
| (1,1003) | 1:A:75:ASN:H | 1:A:75:ASN:HB3 | 5 | 0.15 |
| (1,1) | 1:A:14:LEU:H | 1:A:15:SER:H | 5 | 0.15 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 7 | 0.14 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 1 | 0.14 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 2 | 0.14 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 3 | 0.14 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 6 | 0.14 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 9 | 0.14 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 1 | 0.14 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 8 | 0.14 |
| (1,730) | 1:A:101:LEU:HD11 | 1:A:104:GLN:HG2 | 4 | 0.14 |
| (1,730) | 1:A:101:LEU:HD12 | 1:A:104:GLN:HG2 | 4 | 0.14 |
| (1,730) | 1:A:101:LEU:HD13 | 1:A:104:GLN:HG2 | 4 | 0.14 |
| (1,730) | 1:A:101:LEU:HD21 | 1:A:104:GLN:HG2 | 4 | 0.14 |
| (1,730) | 1:A:101:LEU:HD22 | 1:A:104:GLN:HG2 | 4 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,730) | 1:A:101:LEU:HD23 | 1:A:104:GLN:HG2 | 4 | 0.14 |
| (1,716) | 1:A:71:VAL:HG11 | 1:A:105:LYS:HG2 | 2 | 0.14 |
| (1,716) | 1:A:71:VAL:HG12 | 1:A:105:LYS:HG2 | 2 | 0.14 |
| (1,716) | 1:A:71:VAL:HG13 | 1:A:105:LYS:HG2 | 2 | 0.14 |
| (1,713) | 1:A:10:LEU:HD21 | 1:A:35:GLU:HA | 7 | 0.14 |
| (1,713) | 1:A:10:LEU:HD22 | 1:A:35:GLU:HA | 7 | 0.14 |
| (1,713) | 1:A:10:LEU:HD23 | 1:A:35:GLU:HA | 7 | 0.14 |
| (1,713) | 1:A:10:LEU:HD21 | 1:A:35:GLU:HA | 9 | 0.14 |
| (1,713) | 1:A:10:LEU:HD22 | 1:A:35:GLU:HA | 9 | 0.14 |
| (1,713) | 1:A:10:LEU:HD23 | 1:A:35:GLU:HA | 9 | 0.14 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG21 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG22 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG23 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG21 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG22 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG23 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG21 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG22 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG23 | 2 | 0.14 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG21 | 8 | 0.14 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG22 | 8 | 0.14 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG23 | 8 | 0.14 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG21 | 8 | 0.14 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG22 | 8 | 0.14 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG23 | 8 | 0.14 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG21 | 8 | 0.14 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG22 | 8 | 0.14 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG23 | 8 | 0.14 |
| (1,682) | 1:A:47:ARG:HG3 | 1:A:48:HIS:H | 8 | 0.14 |
| (1,669) | 1:A:61:ARG:HG3 | 1:A:62:PRO:HD2 | 5 | 0.14 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE1 | 3 | 0.14 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE2 | 3 | 0.14 |
| (1,651) | 1:A:46:ILE:HG12 | 1:A:47:ARG:H | 7 | 0.14 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 1 | 0.14 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 1 | 0.14 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 7 | 0.14 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 7 | 0.14 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 10 | 0.14 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 10 | 0.14 |
| (1,633) | 1:A:37:TYR:HA | 1:A:40:ARG:HB2 | 1 | 0.14 |
| (1,58) | 1:A:82:LYS:H | 1:A:82:LYS:HD2 | 7 | 0.14 |
| (1,58) | 1:A:82:LYS:H | 1:A:82:LYS:HD2 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,569) | 1:A:27:ILE:HB | 1:A:30:GLN:HE22 | 6 | 0.14 |
| (1,533) | 1:A:38:ALA:HA | 1:A:43:PHE:HB3 | 9 | 0.14 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD21 | 5 | 0.14 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD22 | 5 | 0.14 |
| (1,522) | 1:A:33:TYR:HB2 | 1:A:34:LEU:HD23 | 5 | 0.14 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD21 | 7 | 0.14 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD22 | 7 | 0.14 |
| (1,520) | 1:A:67:LEU:HB2 | 1:A:79:LEU:HD23 | 7 | 0.14 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD21 | 6 | 0.14 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD22 | 6 | 0.14 |
| (1,506) | 1:A:10:LEU:HB2 | 1:A:34:LEU:HD23 | 6 | 0.14 |
| (1,442) | 1:A:14:LEU:HB2 | 1:A:30:GLN:H | 6 | 0.14 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 2 | 0.14 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 2 | 0.14 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 9 | 0.14 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 9 | 0.14 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 2 | 0.14 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 4 | 0.14 |
| (1,276) | 1:A:26:SER:HB3 | 1:A:27:ILE:H | 2 | 0.14 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 9 | 0.14 |
| (1,256) | 1:A:83:ASP:H | 1:A:86:ARG:HG3 | 10 | 0.14 |
| (1,227) | 1:A:27:ILE:HD11 | 1:A:53:GLY:H | 3 | 0.14 |
| (1,227) | 1:A:27:ILE:HD12 | 1:A:53:GLY:H | 3 | 0.14 |
| (1,227) | 1:A:27:ILE:HD13 | 1:A:53:GLY:H | 3 | 0.14 |
| (1,227) | 1:A:27:ILE:HD11 | 1:A:53:GLY:H | 5 | 0.14 |
| (1,227) | 1:A:27:ILE:HD12 | 1:A:53:GLY:H | 5 | 0.14 |
| (1,227) | 1:A:27:ILE:HD13 | 1:A:53:GLY:H | 5 | 0.14 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG21 | 7 | 0.14 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG22 | 7 | 0.14 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG23 | 7 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG11 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG12 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG13 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG21 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG22 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD1 | 1:A:94:VAL:HG23 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG11 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG12 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG13 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG21 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG22 | 5 | 0.14 |
| (1,1906) | 1:A:59:PHE:HD2 | 1:A:94:VAL:HG23 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1877) | 1:A:12:GLU:HB2 | 1:A:50:THR:HA | 3 | 0.14 |
| (1,1877) | 1:A:12:GLU:HB3 | 1:A:50:THR:HA | 3 | 0.14 |
| (1,1877) | 1:A:12:GLU:HB2 | 1:A:50:THR:HA | 4 | 0.14 |
| (1,1877) | 1:A:12:GLU:HB3 | 1:A:50:THR:HA | 4 | 0.14 |
| (1,1872) | 1:A:91:TYR:HD1 | 1:A:94:VAL:HB | 7 | 0.14 |
| (1,1872) | 1:A:91:TYR:HD2 | 1:A:94:VAL:HB | 7 | 0.14 |
| (1,1839) | 1:A:98:THR:HA | 1:A:102:PHE:HE1 | 5 | 0.14 |
| (1,1839) | 1:A:98:THR:HA | 1:A:102:PHE:HE2 | 5 | 0.14 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD11 | 5 | 0.14 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD12 | 5 | 0.14 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD13 | 5 | 0.14 |
| (1,1830) | 1:A:72:GLU:HA | 1:A:72:GLU:HG2 | 9 | 0.14 |
| (1,1823) | 1:A:32:LYS:HA | 1:A:32:LYS:HG2 | 3 | 0.14 |
| (1,180) | 1:A:54:PHE:H | 1:A:55:SER:H | 3 | 0.14 |
| (1,1789) | 1:A:78:THR:HA | 1:A:108:ARG:HA | 1 | 0.14 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD11 | 10 | 0.14 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD12 | 10 | 0.14 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD13 | 10 | 0.14 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD11 | 10 | 0.14 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD12 | 10 | 0.14 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD13 | 10 | 0.14 |
| (1,1767) | 1:A:7:ILE:HB | 1:A:45:ASN:HD21 | 6 | 0.14 |
| (1,176) | 1:A:66:SER:H | 1:A:67:LEU:HB2 | 6 | 0.14 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 7 | 0.14 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 7 | 0.14 |
| (1,1757) | 1:A:54:PHE:HD1 | 1:A:61:ARG:HA | 8 | 0.14 |
| (1,1757) | 1:A:54:PHE:HD2 | 1:A:61:ARG:HA | 8 | 0.14 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 1 | 0.14 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 1 | 0.14 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD1 | 6 | 0.14 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD2 | 6 | 0.14 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD1 | 6 | 0.14 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD2 | 6 | 0.14 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD1 | 6 | 0.14 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD2 | 6 | 0.14 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD11 | 2 | 0.14 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD12 | 2 | 0.14 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD13 | 2 | 0.14 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 3 | 0.14 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 3 | 0.14 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 3 | 0.14 |
| (1,1596) | 1:A:46:ILE:H | 1:A:46:ILE:HD11 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1596) | 1:A:46:ILE:H | 1:A:46:ILE:HD12 | 5 | 0.14 |
| (1,1596) | 1:A:46:ILE:H | 1:A:46:ILE:HD13 | 5 | 0.14 |
| (1,1589) | 1:A:37:TYR:HD1 | 1:A:110:LEU:HG | 4 | 0.14 |
| (1,1589) | 1:A:37:TYR:HD2 | 1:A:110:LEU:HG | 4 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 2 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 2 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 2 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 2 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 2 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 2 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 10 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 10 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 10 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 10 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 10 | 0.14 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 10 | 0.14 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD11 | 9 | 0.14 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD12 | 9 | 0.14 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD13 | 9 | 0.14 |
| (1,1507) | 1:A:96:PHE:HD1 | 1:A:101:LEU:HG | 4 | 0.14 |
| (1,1507) | 1:A:96:PHE:HD2 | 1:A:101:LEU:HG | 4 | 0.14 |
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 4 | 0.14 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 4 | 0.14 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 4 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 2 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 2 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 6 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 6 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 7 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 7 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 8 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 8 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 9 | 0.14 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 9 | 0.14 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 1 | 0.14 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 5 | 0.14 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 7 | 0.14 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG21 | 9 | 0.14 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG22 | 9 | 0.14 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG23 | 9 | 0.14 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 10 | 0.14 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD11 | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD12 | 9 | 0.14 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD13 | 9 | 0.14 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 3 | 0.14 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 3 | 0.14 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 9 | 0.14 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 9 | 0.14 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE1 | 2 | 0.14 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE2 | 2 | 0.14 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE1 | 4 | 0.14 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE2 | 4 | 0.14 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE1 | 7 | 0.14 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE2 | 7 | 0.14 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD11 | 1 | 0.14 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD12 | 1 | 0.14 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD13 | 1 | 0.14 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD21 | 1 | 0.14 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD22 | 1 | 0.14 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD23 | 1 | 0.14 |
| (1,1390) | 1:A:23:GLU:HA | 1:A:29:ASN:HB2 | 6 | 0.14 |
| (1,1348) | 1:A:31:LYS:HB3 | 1:A:48:HIS:HB3 | 8 | 0.14 |
| (1,1348) | 1:A:31:LYS:HB3 | 1:A:48:HIS:HB3 | 9 | 0.14 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 7 | 0.14 |
| (1,1341) | 1:A:75:ASN:HB3 | 1:A:75:ASN:HD22 | 9 | 0.14 |
| (1,1317) | 1:A:49:PHE:HA | 1:A:50:THR:HB | 1 | 0.14 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 3 | 0.14 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 3 | 0.14 |
| (1,1254) | 1:A:18:ASP:HA | 1:A:20:LEU:HD11 | 5 | 0.14 |
| (1,1254) | 1:A:18:ASP:HA | 1:A:20:LEU:HD12 | 5 | 0.14 |
| (1,1254) | 1:A:18:ASP:HA | 1:A:20:LEU:HD13 | 5 | 0.14 |
| (1,1254) | 1:A:18:ASP:HA | 1:A:20:LEU:HD21 | 5 | 0.14 |
| (1,1254) | 1:A:18:ASP:HA | 1:A:20:LEU:HD22 | 5 | 0.14 |
| (1,1254) | 1:A:18:ASP:HA | 1:A:20:LEU:HD23 | 5 | 0.14 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 3 | 0.14 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 9 | 0.14 |
| (1,1222) | 1:A:93:GLN:HA | 1:A:96:PHE:HD1 | 4 | 0.14 |
| (1,1222) | 1:A:93:GLN:HA | 1:A:96:PHE:HD2 | 4 | 0.14 |
| (1,121) | 1:A:18:ASP:H | 1:A:20:LEU:HG | 8 | 0.14 |
| (1,1174) | 1:A:33:TYR:HE1 | 1:A:82:LYS:HA | 5 | 0.14 |
| (1,1174) | 1:A:33:TYR:HE2 | 1:A:82:LYS:HA | 5 | 0.14 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 3 | 0.14 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 5 | 0.14 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 1 | 0.14 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD1 | 4 | 0.14 |
| (1,1096) | 1:A:38:ALA:HA | 1:A:43:PHE:HD2 | 4 | 0.14 |
| (1,1070) | 1:A:104:GLN:H | 1:A:104:GLN:HB2 | 6 | 0.14 |
| (1,1068) | 1:A:13:ARG:H | 1:A:86:ARG:HG3 | 1 | 0.14 |
| (1,1054) | 1:A:106:ASN:HB2 | 1:A:106:ASN:HD22 | 10 | 0.14 |
| (1,1053) | 1:A:81:VAL:HG21 | 1:A:87:LEU:H | 3 | 0.14 |
| (1,1053) | 1:A:81:VAL:HG22 | 1:A:87:LEU:H | 3 | 0.14 |
| (1,1053) | 1:A:81:VAL:HG23 | 1:A:87:LEU:H | 3 | 0.14 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 6 | 0.14 |
| (1,1047) | 1:A:119:ASN:HA | 1:A:119:ASN:HD22 | 4 | 0.14 |
| (1,998) | 1:A:49:PHE:HB2 | 1:A:67:LEU:H | 5 | 0.13 |
| (1,998) | 1:A:49:PHE:HB2 | 1:A:67:LEU:H | 7 | 0.13 |
| (1,998) | 1:A:49:PHE:HB2 | 1:A:67:LEU:H | 10 | 0.13 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 3 | 0.13 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 6 | 0.13 |
| (1,993) | 1:A:46:ILE:H | 1:A:47:ARG:H | 9 | 0.13 |
| (1,982) | 1:A:43:PHE:H | 1:A:43:PHE:HD1 | 3 | 0.13 |
| (1,982) | 1:A:43:PHE:H | 1:A:43:PHE:HD2 | 3 | 0.13 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 3 | 0.13 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 5 | 0.13 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 6 | 0.13 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 7 | 0.13 |
| (1,860) | 1:A:37:TYR:HB2 | 1:A:38:ALA:H | 10 | 0.13 |
| (1,739) | 1:A:20:LEU:H | 1:A:20:LEU:HD11 | 5 | 0.13 |
| (1,739) | 1:A:20:LEU:H | 1:A:20:LEU:HD12 | 5 | 0.13 |
| (1,739) | 1:A:20:LEU:H | 1:A:20:LEU:HD13 | 5 | 0.13 |
| (1,739) | 1:A:20:LEU:H | 1:A:20:LEU:HD21 | 5 | 0.13 |
| (1,739) | 1:A:20:LEU:H | 1:A:20:LEU:HD22 | 5 | 0.13 |
| (1,739) | 1:A:20:LEU:H | 1:A:20:LEU:HD23 | 5 | 0.13 |
| (1,733) | 1:A:14:LEU:HD11 | 1:A:30:GLN:HE21 | 5 | 0.13 |
| (1,733) | 1:A:14:LEU:HD12 | 1:A:30:GLN:HE21 | 5 | 0.13 |
| (1,733) | 1:A:14:LEU:HD13 | 1:A:30:GLN:HE21 | 5 | 0.13 |
| (1,733) | 1:A:14:LEU:HD21 | 1:A:30:GLN:HE21 | 5 | 0.13 |
| (1,733) | 1:A:14:LEU:HD22 | 1:A:30:GLN:HE21 | 5 | 0.13 |
| (1,733) | 1:A:14:LEU:HD23 | 1:A:30:GLN:HE21 | 5 | 0.13 |
| (1,713) | 1:A:10:LEU:HD21 | 1:A:35:GLU:HA | 4 | 0.13 |
| (1,713) | 1:A:10:LEU:HD22 | 1:A:35:GLU:HA | 4 | 0.13 |
| (1,713) | 1:A:10:LEU:HD23 | 1:A:35:GLU:HA | 4 | 0.13 |
| (1,682) | 1:A:47:ARG:HG3 | 1:A:48:HIS:H | 1 | 0.13 |
| (1,682) | 1:A:47:ARG:HG3 | 1:A:48:HIS:H | 10 | 0.13 |
| (1,654) | 1:A:6:ARG:HG2 | 1:A:7:ILE:H | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,651) | 1:A:46:ILE:HG12 | 1:A:47:ARG:H | 1 | 0.13 |
| (1,651) | 1:A:46:ILE:HG12 | 1:A:47:ARG:H | 2 | 0.13 |
| (1,651) | 1:A:46:ILE:HG12 | 1:A:47:ARG:H | 6 | 0.13 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 2 | 0.13 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 2 | 0.13 |
| (1,633) | 1:A:37:TYR:HA | 1:A:40:ARG:HB2 | 7 | 0.13 |
| (1,572) | 1:A:104:GLN:HA | 1:A:104:GLN:HG3 | 2 | 0.13 |
| (1,563) | 1:A:99:GLU:HA | 1:A:99:GLU:HG2 | 1 | 0.13 |
| (1,559) | 1:A:44:GLU:HG3 | 1:A:45:ASN:HA | 4 | 0.13 |
| (1,557) | 1:A:99:GLU:HA | 1:A:99:GLU:HG3 | 5 | 0.13 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB2 | 1 | 0.13 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB3 | 1 | 0.13 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB2 | 3 | 0.13 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB3 | 3 | 0.13 |
| (1,549) | 1:A:7:ILE:HA | 1:A:45:ASN:HB2 | 2 | 0.13 |
| (1,549) | 1:A:7:ILE:HA | 1:A:45:ASN:HB3 | 2 | 0.13 |
| (1,533) | 1:A:38:ALA:HA | 1:A:43:PHE:HB3 | 4 | 0.13 |
| (1,488) | 1:A:18:ASP:HB2 | 1:A:19:ASP:H | 4 | 0.13 |
| (1,488) | 1:A:18:ASP:HB2 | 1:A:19:ASP:H | 8 | 0.13 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE2 | 2 | 0.13 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE3 | 2 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG11 | 7 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG12 | 7 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG13 | 7 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG21 | 7 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG22 | 7 | 0.13 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG23 | 7 | 0.13 |
| (1,442) | 1:A:14:LEU:HB2 | 1:A:30:GLN:H | 7 | 0.13 |
| (1,438) | 1:A:14:LEU:HB3 | 1:A:30:GLN:H | 2 | 0.13 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 3 | 0.13 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 3 | 0.13 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 10 | 0.13 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 10 | 0.13 |
| (1,419) | 1:A:60:ASN:HA | 1:A:65:GLN:HG2 | 7 | 0.13 |
| (1,419) | 1:A:60:ASN:HA | 1:A:65:GLN:HG3 | 7 | 0.13 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE1 | 1 | 0.13 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE2 | 1 | 0.13 |
| (1,37) | 1:A:52:ASP:H | 1:A:54:PHE:HA | 10 | 0.13 |
| (1,350) | 1:A:69:LYS:HD2 | 1:A:70:GLU:HA | 5 | 0.13 |
| (1,350) | 1:A:69:LYS:HD3 | 1:A:70:GLU:HA | 5 | 0.13 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 1 | 0.13 |
| (1,297) | 1:A:37:TYR:HA | 1:A:39:ARG:HG2 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,284) | 1:A:116:ILE:HG21 | 1:A:118:SER:HB2 | 3 | 0.13 |
| (1,284) | 1:A:116:ILE:HG22 | 1:A:118:SER:HB2 | 3 | 0.13 |
| (1,284) | 1:A:116:ILE:HG23 | 1:A:118:SER:HB2 | 3 | 0.13 |
| (1,269) | 1:A:71:VAL:HA | 1:A:76:VAL:HB | 4 | 0.13 |
| (1,243) | 1:A:70:GLU:HA | 1:A:75:ASN:HD22 | 1 | 0.13 |
| (1,229) | 1:A:39:ARG:HG2 | 1:A:41:ASN:H | 2 | 0.13 |
| (1,222) | 1:A:83:ASP:HA | 1:A:85:SER:H | 8 | 0.13 |
| (1,221) | 1:A:13:ARG:HH12 | 1:A:85:SER:H | 2 | 0.13 |
| (1,221) | 1:A:13:ARG:HH12 | 1:A:85:SER:H | 3 | 0.13 |
| (1,221) | 1:A:13:ARG:HH12 | 1:A:85:SER:H | 7 | 0.13 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG21 | 2 | 0.13 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG22 | 2 | 0.13 |
| (1,21) | 1:A:9:ALA:H | 1:A:78:THR:HG23 | 2 | 0.13 |
| (1,205) | 1:A:26:SER:H | 1:A:30:GLN:HE22 | 6 | 0.13 |
| (1,1928) | 1:A:107:VAL:HG21 | 1:A:109:PHE:HB3 | 2 | 0.13 |
| (1,1928) | 1:A:107:VAL:HG22 | 1:A:109:PHE:HB3 | 2 | 0.13 |
| (1,1928) | 1:A:107:VAL:HG23 | 1:A:109:PHE:HB3 | 2 | 0.13 |
| (1,1928) | 1:A:107:VAL:HG21 | 1:A:109:PHE:HB3 | 4 | 0.13 |
| (1,1928) | 1:A:107:VAL:HG22 | 1:A:109:PHE:HB3 | 4 | 0.13 |
| (1,1928) | 1:A:107:VAL:HG23 | 1:A:109:PHE:HB3 | 4 | 0.13 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 4 | 0.13 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 4 | 0.13 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 4 | 0.13 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 10 | 0.13 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 10 | 0.13 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 10 | 0.13 |
| (1,1872) | 1:A:91:TYR:HD1 | 1:A:94:VAL:HB | 5 | 0.13 |
| (1,1872) | 1:A:91:TYR:HD2 | 1:A:94:VAL:HB | 5 | 0.13 |
| (1,1872) | 1:A:91:TYR:HD1 | 1:A:94:VAL:HB | 8 | 0.13 |
| (1,1872) | 1:A:91:TYR:HD2 | 1:A:94:VAL:HB | 8 | 0.13 |
| (1,1869) | 1:A:57:VAL:HB | 1:A:58:ASN:HD22 | 10 | 0.13 |
| (1,1853) | 1:A:47:ARG:HA | 1:A:47:ARG:HD2 | 4 | 0.13 |
| (1,1853) | 1:A:47:ARG:HA | 1:A:47:ARG:HD3 | 4 | 0.13 |
| (1,1837) | 1:A:28:THR:HA | 1:A:31:LYS:HD2 | 4 | 0.13 |
| (1,180) | 1:A:54:PHE:H | 1:A:55:SER:H | 4 | 0.13 |
| (1,180) | 1:A:54:PHE:H | 1:A:55:SER:H | 6 | 0.13 |
| (1,1792) | 1:A:13:ARG:HA | 1:A:54:PHE:HD1 | 3 | 0.13 |
| (1,1792) | 1:A:13:ARG:HA | 1:A:54:PHE:HD2 | 3 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD11 | 8 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD12 | 8 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD13 | 8 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD11 | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD12 | 8 | 0.13 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD13 | 8 | 0.13 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD1 | 4 | 0.13 |
| (1,1770) | 1:A:34:LEU:HA | 1:A:37:TYR:HD2 | 4 | 0.13 |
| (1,176) | 1:A:66:SER:H | 1:A:67:LEU:HB2 | 2 | 0.13 |
| (1,176) | 1:A:66:SER:H | 1:A:67:LEU:HB2 | 7 | 0.13 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 7 | 0.13 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 7 | 0.13 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 9 | 0.13 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 9 | 0.13 |
| (1,1729) | 1:A:49:PHE:HE1 | 1:A:7:ILE:HD11 | 9 | 0.13 |
| (1,1729) | 1:A:49:PHE:HE1 | 1:A:7:ILE:HD12 | 9 | 0.13 |
| (1,1729) | 1:A:49:PHE:HE1 | 1:A:7:ILE:HD13 | 9 | 0.13 |
| (1,1729) | 1:A:49:PHE:HE2 | 1:A:7:ILE:HD11 | 9 | 0.13 |
| (1,1729) | 1:A:49:PHE:HE2 | 1:A:7:ILE:HD12 | 9 | 0.13 |
| (1,1729) | 1:A:49:PHE:HE2 | 1:A:7:ILE:HD13 | 9 | 0.13 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD1 | 7 | 0.13 |
| (1,1724) | 1:A:81:VAL:HG21 | 1:A:109:PHE:HD2 | 7 | 0.13 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD1 | 7 | 0.13 |
| (1,1724) | 1:A:81:VAL:HG22 | 1:A:109:PHE:HD2 | 7 | 0.13 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD1 | 7 | 0.13 |
| (1,1724) | 1:A:81:VAL:HG23 | 1:A:109:PHE:HD2 | 7 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD1 | 7 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD2 | 7 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD1 | 7 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD2 | 7 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD1 | 7 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD2 | 7 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD1 | 8 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD2 | 8 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD1 | 8 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD2 | 8 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD1 | 8 | 0.13 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD2 | 8 | 0.13 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD11 | 6 | 0.13 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD12 | 6 | 0.13 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD13 | 6 | 0.13 |
| (1,168) | 1:A:103:PRO:HD3 | 1:A:104:GLN:H | 3 | 0.13 |
| (1,168) | 1:A:103:PRO:HD3 | 1:A:104:GLN:H | 4 | 0.13 |
| (1,168) | 1:A:103:PRO:HD3 | 1:A:104:GLN:H | 9 | 0.13 |
| (1,168) | 1:A:103:PRO:HD3 | 1:A:104:GLN:H | 10 | 0.13 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 8 | 0.13 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 8 | 0.13 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 8 | 0.13 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 8 | 0.13 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 8 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD21 | 4 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD22 | 4 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD23 | 4 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD21 | 4 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD22 | 4 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD23 | 4 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD21 | 4 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD22 | 4 | 0.13 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD23 | 4 | 0.13 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD21 | 4 | 0.13 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD22 | 4 | 0.13 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD23 | 4 | 0.13 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD21 | 8 | 0.13 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD22 | 8 | 0.13 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD23 | 8 | 0.13 |
| (1,1589) | 1:A:37:TYR:HD1 | 1:A:110:LEU:HG | 7 | 0.13 |
| (1,1589) | 1:A:37:TYR:HD2 | 1:A:110:LEU:HG | 7 | 0.13 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD11 | 4 | 0.13 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD12 | 4 | 0.13 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD13 | 4 | 0.13 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD21 | 4 | 0.13 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD22 | 4 | 0.13 |
| (1,1566) | 1:A:17:ASP:H | 1:A:20:LEU:HD23 | 4 | 0.13 |
| (1,1507) | 1:A:96:PHE:HD1 | 1:A:101:LEU:HG | 1 | 0.13 |
| (1,1507) | 1:A:96:PHE:HD2 | 1:A:101:LEU:HG | 1 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB1 | 6 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB2 | 6 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB3 | 6 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB1 | 6 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB2 | 6 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB3 | 6 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB1 | 9 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB2 | 9 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB3 | 9 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB1 | 9 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB2 | 9 | 0.13 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB3 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 3 | 0.13 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 3 | 0.13 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 3 | 0.13 |
| (1,1494) | 1:A:50:THR:HG21 | 1:A:63:GLY:HA2 | 2 | 0.13 |
| (1,1494) | 1:A:50:THR:HG22 | 1:A:63:GLY:HA2 | 2 | 0.13 |
| (1,1494) | 1:A:50:THR:HG23 | 1:A:63:GLY:HA2 | 2 | 0.13 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG21 | 1 | 0.13 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG22 | 1 | 0.13 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG23 | 1 | 0.13 |
| (1,1440) | 1:A:6:ARG:HG3 | 1:A:75:ASN:HA | 9 | 0.13 |
| (1,1432) | 1:A:34:LEU:H | 1:A:34:LEU:HB3 | 9 | 0.13 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 5 | 0.13 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 7 | 0.13 |
| (1,1414) | 1:A:44:GLU:H | 1:A:44:GLU:HG3 | 2 | 0.13 |
| (1,1414) | 1:A:44:GLU:H | 1:A:44:GLU:HG3 | 3 | 0.13 |
| (1,1414) | 1:A:44:GLU:H | 1:A:44:GLU:HG3 | 9 | 0.13 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD11 | 10 | 0.13 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD12 | 10 | 0.13 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD13 | 10 | 0.13 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 1 | 0.13 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 1 | 0.13 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 2 | 0.13 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 2 | 0.13 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE1 | 6 | 0.13 |
| (1,1401) | 1:A:97:TYR:HB3 | 1:A:109:PHE:HE2 | 6 | 0.13 |
| (1,1399) | 1:A:70:GLU:HA | 1:A:72:GLU:HG3 | 3 | 0.13 |
| (1,1399) | 1:A:70:GLU:HA | 1:A:72:GLU:HG3 | 10 | 0.13 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG21 | 3 | 0.13 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG22 | 3 | 0.13 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG23 | 3 | 0.13 |
| (1,1383) | 1:A:103:PRO:HA | 1:A:106:ASN:HB2 | 3 | 0.13 |
| (1,1383) | 1:A:103:PRO:HA | 1:A:106:ASN:HB2 | 7 | 0.13 |
| (1,1348) | 1:A:31:LYS:HB3 | 1:A:48:HIS:HB3 | 10 | 0.13 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 4 | 0.13 |
| (1,1340) | 1:A:7:ILE:HB | 1:A:75:ASN:HB3 | 6 | 0.13 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD1 | 5 | 0.13 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD2 | 5 | 0.13 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD1 | 10 | 0.13 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD2 | 10 | 0.13 |
| (1,1323) | 1:A:71:VAL:HA | 1:A:105:LYS:HG2 | 5 | 0.13 |
| (1,1323) | 1:A:71:VAL:HA | 1:A:105:LYS:HG2 | 8 | 0.13 |
| (1,1300) | 1:A:78:THR:HG21 | 1:A:107:VAL:HA | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1300) | 1:A:78:THR:HG22 | 1:A:107:VAL:HA | 9 | 0.13 |
| (1,1300) | 1:A:78:THR:HG23 | 1:A:107:VAL:HA | 9 | 0.13 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 1 | 0.13 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 1 | 0.13 |
| (1,1253) | 1:A:83:ASP:HA | 1:A:111:ALA:HA | 2 | 0.13 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 4 | 0.13 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 5 | 0.13 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 2 | 0.13 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 4 | 0.13 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 9 | 0.13 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 10 | 0.13 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 4 | 0.13 |
| (1,1116) | 1:A:5:SER:HA | 1:A:45:ASN:HD22 | 1 | 0.13 |
| (1,1116) | 1:A:5:SER:HA | 1:A:45:ASN:HD22 | 4 | 0.13 |
| (1,1116) | 1:A:5:SER:HA | 1:A:45:ASN:HD22 | 8 | 0.13 |
| (1,1109) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HE1 | 8 | 0.13 |
| (1,1109) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HE2 | 8 | 0.13 |
| (1,1103) | 1:A:41:ASN:H | 1:A:41:ASN:HB3 | 1 | 0.13 |
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD11 | 7 | 0.13 |
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD12 | 7 | 0.13 |
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD13 | 7 | 0.13 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD11 | 7 | 0.13 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD12 | 7 | 0.13 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD13 | 7 | 0.13 |
| (1,1068) | 1:A:13:ARG:H | 1:A:86:ARG:HG3 | 8 | 0.13 |
| (1,1054) | 1:A:106:ASN:HB2 | 1:A:106:ASN:HD22 | 9 | 0.13 |
| (1,1053) | 1:A:81:VAL:HG21 | 1:A:87:LEU:H | 6 | 0.13 |
| (1,1053) | 1:A:81:VAL:HG22 | 1:A:87:LEU:H | 6 | 0.13 |
| (1,1053) | 1:A:81:VAL:HG23 | 1:A:87:LEU:H | 6 | 0.13 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 1 | 0.13 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 3 | 0.13 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 7 | 0.13 |
| (1,1011) | 1:A:32:LYS:H | 1:A:48:HIS:HE1 | 2 | 0.13 |
| (1,1011) | 1:A:32:LYS:H | 1:A:48:HIS:HE1 | 10 | 0.13 |
| (1,1) | 1:A:14:LEU:H | 1:A:15:SER:H | 3 | 0.13 |
| (1,998) | 1:A:49:PHE:HB2 | 1:A:67:LEU:H | 9 | 0.12 |
| (1,982) | 1:A:43:PHE:H | 1:A:43:PHE:HD1 | 5 | 0.12 |
| (1,982) | 1:A:43:PHE:H | 1:A:43:PHE:HD2 | 5 | 0.12 |
| (1,969) | 1:A:19:ASP:H | 1:A:19:ASP:HA | 1 | 0.12 |
| (1,969) | 1:A:19:ASP:H | 1:A:19:ASP:HA | 4 | 0.12 |
| (1,969) | 1:A:19:ASP:H | 1:A:19:ASP:HA | 9 | 0.12 |
| (1,88) | 1:A:119:ASN:H | 1:A:120:ASN:H | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 4 | 0.12 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 7 | 0.12 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 8 | 0.12 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 10 | 0.12 |
| (1,733) | 1:A:14:LEU:HD11 | 1:A:30:GLN:HE21 | 3 | 0.12 |
| (1,733) | 1:A:14:LEU:HD12 | 1:A:30:GLN:HE21 | 3 | 0.12 |
| (1,733) | 1:A:14:LEU:HD13 | 1:A:30:GLN:HE21 | 3 | 0.12 |
| (1,733) | 1:A:14:LEU:HD21 | 1:A:30:GLN:HE21 | 3 | 0.12 |
| (1,733) | 1:A:14:LEU:HD22 | 1:A:30:GLN:HE21 | 3 | 0.12 |
| (1,733) | 1:A:14:LEU:HD23 | 1:A:30:GLN:HE21 | 3 | 0.12 |
| (1,733) | 1:A:14:LEU:HD11 | 1:A:30:GLN:HE21 | 6 | 0.12 |
| (1,733) | 1:A:14:LEU:HD12 | 1:A:30:GLN:HE21 | 6 | 0.12 |
| (1,733) | 1:A:14:LEU:HD13 | 1:A:30:GLN:HE21 | 6 | 0.12 |
| (1,733) | 1:A:14:LEU:HD21 | 1:A:30:GLN:HE21 | 6 | 0.12 |
| (1,733) | 1:A:14:LEU:HD22 | 1:A:30:GLN:HE21 | 6 | 0.12 |
| (1,733) | 1:A:14:LEU:HD23 | 1:A:30:GLN:HE21 | 6 | 0.12 |
| (1,682) | 1:A:47:ARG:HG3 | 1:A:48:HIS:H | 2 | 0.12 |
| (1,666) | 1:A:81:VAL:HG21 | 1:A:87:LEU:HG | 10 | 0.12 |
| (1,666) | 1:A:81:VAL:HG22 | 1:A:87:LEU:HG | 10 | 0.12 |
| (1,666) | 1:A:81:VAL:HG23 | 1:A:87:LEU:HG | 10 | 0.12 |
| (1,665) | 1:A:61:ARG:HA | 1:A:62:PRO:HG3 | 1 | 0.12 |
| (1,633) | 1:A:37:TYR:HA | 1:A:40:ARG:HB2 | 4 | 0.12 |
| (1,633) | 1:A:37:TYR:HA | 1:A:40:ARG:HB2 | 10 | 0.12 |
| (1,620) | 1:A:103:PRO:HB3 | 1:A:104:GLN:H | 1 | 0.12 |
| (1,620) | 1:A:103:PRO:HB3 | 1:A:104:GLN:H | 5 | 0.12 |
| (1,620) | 1:A:103:PRO:HB3 | 1:A:104:GLN:H | 9 | 0.12 |
| (1,58) | 1:A:82:LYS:H | 1:A:82:LYS:HD2 | 5 | 0.12 |
| (1,572) | 1:A:104:GLN:HA | 1:A:104:GLN:HG3 | 5 | 0.12 |
| (1,563) | 1:A:99:GLU:HA | 1:A:99:GLU:HG2 | 4 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB2 | 2 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB3 | 2 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB2 | 7 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB3 | 7 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB2 | 9 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB3 | 9 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB2 | 10 | 0.12 |
| (1,550) | 1:A:44:GLU:HA | 1:A:45:ASN:HB3 | 10 | 0.12 |
| (1,549) | 1:A:7:ILE:HA | 1:A:45:ASN:HB2 | 9 | 0.12 |
| (1,549) | 1:A:7:ILE:HA | 1:A:45:ASN:HB3 | 9 | 0.12 |
| (1,549) | 1:A:7:ILE:HA | 1:A:45:ASN:HB2 | 10 | 0.12 |
| (1,549) | 1:A:7:ILE:HA | 1:A:45:ASN:HB3 | 10 | 0.12 |
| (1,545) | 1:A:35:GLU:H | 1:A:35:GLU:HG3 | 3 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,545) | 1:A:35:GLU:H | 1:A:35:GLU:HG3 | 8 | 0.12 |
| (1,533) | 1:A:38:ALA:HA | 1:A:43:PHE:HB3 | 1 | 0.12 |
| (1,533) | 1:A:38:ALA:HA | 1:A:43:PHE:HB3 | 10 | 0.12 |
| (1,532) | 1:A:8:THR:HB | 1:A:46:ILE:HB | 10 | 0.12 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 1 | 0.12 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 6 | 0.12 |
| (1,495) | 1:A:7:ILE:HB | 1:A:76:VAL:HA | 10 | 0.12 |
| (1,488) | 1:A:18:ASP:HB2 | 1:A:19:ASP:H | 3 | 0.12 |
| (1,488) | 1:A:18:ASP:HB2 | 1:A:19:ASP:H | 9 | 0.12 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE2 | 7 | 0.12 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE3 | 7 | 0.12 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE2 | 9 | 0.12 |
| (1,474) | 1:A:105:LYS:HA | 1:A:105:LYS:HE3 | 9 | 0.12 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG11 | 10 | 0.12 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG12 | 10 | 0.12 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG13 | 10 | 0.12 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG21 | 10 | 0.12 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG22 | 10 | 0.12 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG23 | 10 | 0.12 |
| (1,447) | 1:A:95:GLY:HA3 | 1:A:99:GLU:H | 3 | 0.12 |
| (1,438) | 1:A:14:LEU:HB3 | 1:A:30:GLN:H | 3 | 0.12 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 4 | 0.12 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 4 | 0.12 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 5 | 0.12 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 5 | 0.12 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 8 | 0.12 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 8 | 0.12 |
| (1,419) | 1:A:60:ASN:HA | 1:A:65:GLN:HG2 | 4 | 0.12 |
| (1,419) | 1:A:60:ASN:HA | 1:A:65:GLN:HG3 | 4 | 0.12 |
| (1,406) | 1:A:41:ASN:HA | 1:A:42:GLY:H | 6 | 0.12 |
| (1,406) | 1:A:41:ASN:HA | 1:A:42:GLY:H | 7 | 0.12 |
| (1,406) | 1:A:41:ASN:HA | 1:A:42:GLY:H | 10 | 0.12 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE1 | 2 | 0.12 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE2 | 2 | 0.12 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE1 | 8 | 0.12 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE2 | 8 | 0.12 |
| (1,371) | 1:A:92:LEU:HA | 1:A:92:LEU:HD11 | 10 | 0.12 |
| (1,371) | 1:A:92:LEU:HA | 1:A:92:LEU:HD12 | 10 | 0.12 |
| (1,371) | 1:A:92:LEU:HA | 1:A:92:LEU:HD13 | 10 | 0.12 |
| (1,347) | 1:A:116:ILE:HG21 | 1:A:118:SER:HA | 6 | 0.12 |
| (1,347) | 1:A:116:ILE:HG22 | 1:A:118:SER:HA | 6 | 0.12 |
| (1,347) | 1:A:116:ILE:HG23 | 1:A:118:SER:HA | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,303) | 1:A:10:LEU:H | 1:A:46:ILE:HA | 7 | 0.12 |
| (1,303) | 1:A:10:LEU:H | 1:A:46:ILE:HA | 9 | 0.12 |
| (1,263) | 1:A:8:THR:HB | 1:A:45:ASN:HA | 5 | 0.12 |
| (1,227) | 1:A:27:ILE:HD11 | 1:A:53:GLY:H | 7 | 0.12 |
| (1,227) | 1:A:27:ILE:HD12 | 1:A:53:GLY:H | 7 | 0.12 |
| (1,227) | 1:A:27:ILE:HD13 | 1:A:53:GLY:H | 7 | 0.12 |
| (1,221) | 1:A:13:ARG:HH12 | 1:A:85:SER:H | 5 | 0.12 |
| (1,205) | 1:A:26:SER:H | 1:A:30:GLN:HE22 | 9 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD11 | 2 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD12 | 2 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD13 | 2 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD11 | 4 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD12 | 4 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD13 | 4 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD11 | 9 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD12 | 9 | 0.12 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD13 | 9 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD11 | 1:A:18:ASP:HB2 | 3 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD12 | 1:A:18:ASP:HB2 | 3 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD13 | 1:A:18:ASP:HB2 | 3 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD21 | 1:A:18:ASP:HB2 | 3 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD22 | 1:A:18:ASP:HB2 | 3 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD23 | 1:A:18:ASP:HB2 | 3 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD11 | 1:A:18:ASP:HB2 | 7 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD12 | 1:A:18:ASP:HB2 | 7 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD13 | 1:A:18:ASP:HB2 | 7 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD21 | 1:A:18:ASP:HB2 | 7 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD22 | 1:A:18:ASP:HB2 | 7 | 0.12 |
| (1,1901) | 1:A:14:LEU:HD23 | 1:A:18:ASP:HB2 | 7 | 0.12 |
| (1,1877) | 1:A:12:GLU:HB2 | 1:A:50:THR:HA | 7 | 0.12 |
| (1,1877) | 1:A:12:GLU:HB3 | 1:A:50:THR:HA | 7 | 0.12 |
| (1,1872) | 1:A:91:TYR:HD1 | 1:A:94:VAL:HB | 2 | 0.12 |
| (1,1872) | 1:A:91:TYR:HD2 | 1:A:94:VAL:HB | 2 | 0.12 |
| (1,1870) | 1:A:44:GLU:HA | 1:A:44:GLU:HG2 | 7 | 0.12 |
| (1,1857) | 1:A:104:GLN:HB3 | 1:A:105:LYS:HE2 | 5 | 0.12 |
| (1,1857) | 1:A:104:GLN:HB3 | 1:A:105:LYS:HE3 | 5 | 0.12 |
| (1,1854) | 1:A:47:ARG:HD2 | 1:A:49:PHE:HA | 4 | 0.12 |
| (1,1854) | 1:A:47:ARG:HD3 | 1:A:49:PHE:HA | 4 | 0.12 |
| (1,1853) | 1:A:47:ARG:HA | 1:A:47:ARG:HD2 | 10 | 0.12 |
| (1,1853) | 1:A:47:ARG:HA | 1:A:47:ARG:HD3 | 10 | 0.12 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG11 | 1 | 0.12 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG12 | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG13 | 1 | 0.12 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG21 | 1 | 0.12 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG22 | 1 | 0.12 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG23 | 1 | 0.12 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD11 | 2 | 0.12 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD12 | 2 | 0.12 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD13 | 2 | 0.12 |
| (1,1819) | 1:A:40:ARG:HA | 1:A:40:ARG:HB3 | 9 | 0.12 |
| (1,1807) | 1:A:23:GLU:HA | 1:A:23:GLU:HG2 | 3 | 0.12 |
| (1,1807) | 1:A:23:GLU:HA | 1:A:23:GLU:HG3 | 3 | 0.12 |
| (1,180) | 1:A:54:PHE:H | 1:A:55:SER:H | 7 | 0.12 |
| (1,1789) | 1:A:78:THR:HA | 1:A:108:ARG:HA | 5 | 0.12 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 6 | 0.12 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 6 | 0.12 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 8 | 0.12 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 8 | 0.12 |
| (1,1785) | 1:A:50:THR:HA | 1:A:54:PHE:HZ | 3 | 0.12 |
| (1,1785) | 1:A:50:THR:HA | 1:A:54:PHE:HZ | 10 | 0.12 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD11 | 6 | 0.12 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD12 | 6 | 0.12 |
| (1,1778) | 1:A:59:PHE:HD1 | 1:A:68:ILE:HD13 | 6 | 0.12 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD11 | 6 | 0.12 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD12 | 6 | 0.12 |
| (1,1778) | 1:A:59:PHE:HD2 | 1:A:68:ILE:HD13 | 6 | 0.12 |
| (1,1765) | 1:A:30:GLN:HE22 | 1:A:31:LYS:HA | 8 | 0.12 |
| (1,1765) | 1:A:30:GLN:HE22 | 1:A:31:LYS:HA | 9 | 0.12 |
| (1,176) | 1:A:66:SER:H | 1:A:67:LEU:HB2 | 1 | 0.12 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 6 | 0.12 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 6 | 0.12 |
| (1,1742) | 1:A:34:LEU:HD21 | 1:A:48:HIS:HE1 | 2 | 0.12 |
| (1,1742) | 1:A:34:LEU:HD22 | 1:A:48:HIS:HE1 | 2 | 0.12 |
| (1,1742) | 1:A:34:LEU:HD23 | 1:A:48:HIS:HE1 | 2 | 0.12 |
| (1,1740) | 1:A:31:LYS:HA | 1:A:48:HIS:HE1 | 1 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD11 | 3 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD12 | 3 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD13 | 3 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD11 | 4 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD12 | 4 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD13 | 4 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD11 | 7 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD12 | 7 | 0.12 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD13 | 7 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD11 | 4 | 0.12 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD12 | 4 | 0.12 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD13 | 4 | 0.12 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD11 | 8 | 0.12 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD12 | 8 | 0.12 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD13 | 8 | 0.12 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD11 | 2 | 0.12 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD12 | 2 | 0.12 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD13 | 2 | 0.12 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD11 | 6 | 0.12 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD12 | 6 | 0.12 |
| (1,1658) | 1:A:11:TYR:HA | 1:A:79:LEU:HD13 | 6 | 0.12 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE1 | 2 | 0.12 |
| (1,1657) | 1:A:79:LEU:HD11 | 1:A:102:PHE:HE2 | 2 | 0.12 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE1 | 2 | 0.12 |
| (1,1657) | 1:A:79:LEU:HD12 | 1:A:102:PHE:HE2 | 2 | 0.12 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE1 | 2 | 0.12 |
| (1,1657) | 1:A:79:LEU:HD13 | 1:A:102:PHE:HE2 | 2 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD11 | 1 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD12 | 1 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD13 | 1 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD11 | 4 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD12 | 4 | 0.12 |
| (1,1599) | 1:A:35:GLU:HG3 | 1:A:46:ILE:HD13 | 4 | 0.12 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD11 | 9 | 0.12 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD12 | 9 | 0.12 |
| (1,1593) | 1:A:39:ARG:HD2 | 1:A:46:ILE:HD13 | 9 | 0.12 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD11 | 9 | 0.12 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD12 | 9 | 0.12 |
| (1,1593) | 1:A:39:ARG:HD3 | 1:A:46:ILE:HD13 | 9 | 0.12 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG21 | 10 | 0.12 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG22 | 10 | 0.12 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG23 | 10 | 0.12 |
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 3 | 0.12 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 3 | 0.12 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 3 | 0.12 |
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 5 | 0.12 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 5 | 0.12 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 5 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB1 | 3 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB2 | 3 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB3 | 3 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB1 | 3 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB2 | 3 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB3 | 3 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB1 | 4 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB2 | 4 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB3 | 4 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB1 | 4 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB2 | 4 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB3 | 4 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB1 | 7 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB2 | 7 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE1 | 1:A:111:ALA:HB3 | 7 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB1 | 7 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB2 | 7 | 0.12 |
| (1,1501) | 1:A:109:PHE:HE2 | 1:A:111:ALA:HB3 | 7 | 0.12 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD1 | 4 | 0.12 |
| (1,15) | 1:A:108:ARG:H | 1:A:109:PHE:HD2 | 4 | 0.12 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 4 | 0.12 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 6 | 0.12 |
| (1,1498) | 1:A:110:LEU:HB2 | 1:A:111:ALA:H | 8 | 0.12 |
| (1,1470) | 1:A:74:GLY:HA3 | 1:A:105:LYS:HG2 | 9 | 0.12 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 6 | 0.12 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 9 | 0.12 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD11 | 6 | 0.12 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD12 | 6 | 0.12 |
| (1,141) | 1:A:13:ARG:H | 1:A:27:ILE:HD13 | 6 | 0.12 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 5 | 0.12 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 5 | 0.12 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG21 | 2 | 0.12 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG22 | 2 | 0.12 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG23 | 2 | 0.12 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG21 | 7 | 0.12 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG22 | 7 | 0.12 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG23 | 7 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD11 | 3 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD12 | 3 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD13 | 3 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD21 | 3 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD22 | 3 | 0.12 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD23 | 3 | 0.12 |
| (1,1390) | 1:A:23:GLU:HA | 1:A:29:ASN:HB2 | 1 | 0.12 |
| (1,1390) | 1:A:23:GLU:HA | 1:A:29:ASN:HB2 | 7 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1383) | 1:A:103:PRO:HA | 1:A:106:ASN:HB2 | 1 | 0.12 |
| (1,1383) | 1:A:103:PRO:HA | 1:A:106:ASN:HB2 | 6 | 0.12 |
| (1,1348) | 1:A:31:LYS:HB3 | 1:A:48:HIS:HB3 | 1 | 0.12 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 2 | 0.12 |
| (1,1343) | 1:A:70:GLU:HA | 1:A:75:ASN:HB3 | 10 | 0.12 |
| (1,1340) | 1:A:7:ILE:HB | 1:A:75:ASN:HB3 | 3 | 0.12 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD1 | 7 | 0.12 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD2 | 7 | 0.12 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD1 | 8 | 0.12 |
| (1,1325) | 1:A:98:THR:HA | 1:A:102:PHE:HD2 | 8 | 0.12 |
| (1,1323) | 1:A:71:VAL:HA | 1:A:105:LYS:HG2 | 1 | 0.12 |
| (1,1303) | 1:A:102:PHE:HD1 | 1:A:107:VAL:HA | 5 | 0.12 |
| (1,1303) | 1:A:102:PHE:HD2 | 1:A:107:VAL:HA | 5 | 0.12 |
| (1,1300) | 1:A:78:THR:HG21 | 1:A:107:VAL:HA | 2 | 0.12 |
| (1,1300) | 1:A:78:THR:HG22 | 1:A:107:VAL:HA | 2 | 0.12 |
| (1,1300) | 1:A:78:THR:HG23 | 1:A:107:VAL:HA | 2 | 0.12 |
| (1,1300) | 1:A:78:THR:HG21 | 1:A:107:VAL:HA | 3 | 0.12 |
| (1,1300) | 1:A:78:THR:HG22 | 1:A:107:VAL:HA | 3 | 0.12 |
| (1,1300) | 1:A:78:THR:HG23 | 1:A:107:VAL:HA | 3 | 0.12 |
| (1,1298) | 1:A:33:TYR:HE1 | 1:A:34:LEU:HA | 5 | 0.12 |
| (1,1298) | 1:A:33:TYR:HE2 | 1:A:34:LEU:HA | 5 | 0.12 |
| (1,1284) | 1:A:104:GLN:HA | 1:A:104:GLN:HB2 | 5 | 0.12 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 1 | 0.12 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 3 | 0.12 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 6 | 0.12 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 7 | 0.12 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 8 | 0.12 |
| (1,1214) | 1:A:58:ASN:HA | 1:A:59:PHE:HD1 | 2 | 0.12 |
| (1,1214) | 1:A:58:ASN:HA | 1:A:59:PHE:HD2 | 2 | 0.12 |
| (1,1214) | 1:A:58:ASN:HA | 1:A:59:PHE:HD1 | 10 | 0.12 |
| (1,1214) | 1:A:58:ASN:HA | 1:A:59:PHE:HD2 | 10 | 0.12 |
| (1,1213) | 1:A:102:PHE:H | 1:A:102:PHE:HE1 | 6 | 0.12 |
| (1,1213) | 1:A:102:PHE:H | 1:A:102:PHE:HE2 | 6 | 0.12 |
| (1,1194) | 1:A:61:ARG:HG2 | 1:A:64:PHE:HE1 | 9 | 0.12 |
| (1,1194) | 1:A:61:ARG:HG2 | 1:A:64:PHE:HE2 | 9 | 0.12 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 1 | 0.12 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 1 | 0.12 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 6 | 0.12 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 6 | 0.12 |
| (1,116) | 1:A:37:TYR:H | 1:A:39:ARG:H | 1 | 0.12 |
| (1,113) | 1:A:44:GLU:H | 1:A:44:GLU:HG2 | 6 | 0.12 |
| (1,1116) | 1:A:5:SER:HA | 1:A:45:ASN:HD22 | 7 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1109) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HE1 | 2 | 0.12 |
| (1,1109) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HE2 | 2 | 0.12 |
| (1,1103) | 1:A:41:ASN:H | 1:A:41:ASN:HB3 | 9 | 0.12 |
| (1,1103) | 1:A:41:ASN:H | 1:A:41:ASN:HB3 | 10 | 0.12 |
| (1,1070) | 1:A:104:GLN:H | 1:A:104:GLN:HB2 | 1 | 0.12 |
| (1,1068) | 1:A:13:ARG:H | 1:A:86:ARG:HG3 | 3 | 0.12 |
| (1,1053) | 1:A:81:VAL:HG21 | 1:A:87:LEU:H | 4 | 0.12 |
| (1,1053) | 1:A:81:VAL:HG22 | 1:A:87:LEU:H | 4 | 0.12 |
| (1,1053) | 1:A:81:VAL:HG23 | 1:A:87:LEU:H | 4 | 0.12 |
| (1,1053) | 1:A:81:VAL:HG21 | 1:A:87:LEU:H | 5 | 0.12 |
| (1,1053) | 1:A:81:VAL:HG22 | 1:A:87:LEU:H | 5 | 0.12 |
| (1,1053) | 1:A:81:VAL:HG23 | 1:A:87:LEU:H | 5 | 0.12 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 2 | 0.12 |
| (1,1049) | 1:A:119:ASN:HB2 | 1:A:119:ASN:HD22 | 8 | 0.12 |
| (1,1013) | 1:A:35:GLU:HG2 | 1:A:48:HIS:HE1 | 2 | 0.12 |
| (1,1011) | 1:A:32:LYS:H | 1:A:48:HIS:HE1 | 4 | 0.12 |
| (1,1003) | 1:A:75:ASN:H | 1:A:75:ASN:HB3 | 8 | 0.12 |
| (1,1003) | 1:A:75:ASN:H | 1:A:75:ASN:HB3 | 10 | 0.12 |
| (1,998) | 1:A:49:PHE:HB2 | 1:A:67:LEU:H | 1 | 0.11 |
| (1,998) | 1:A:49:PHE:HB2 | 1:A:67:LEU:H | 8 | 0.11 |
| (1,969) | 1:A:19:ASP:H | 1:A:19:ASP:HA | 3 | 0.11 |
| (1,916) | 1:A:36:ASP:H | 1:A:36:ASP:HB3 | 8 | 0.11 |
| (1,862) | 1:A:79:LEU:HB2 | 1:A:80:ILE:H | 5 | 0.11 |
| (1,716) | 1:A:71:VAL:HG11 | 1:A:105:LYS:HG2 | 7 | 0.11 |
| (1,716) | 1:A:71:VAL:HG12 | 1:A:105:LYS:HG2 | 7 | 0.11 |
| (1,716) | 1:A:71:VAL:HG13 | 1:A:105:LYS:HG2 | 7 | 0.11 |
| (1,713) | 1:A:10:LEU:HD21 | 1:A:35:GLU:HA | 1 | 0.11 |
| (1,713) | 1:A:10:LEU:HD22 | 1:A:35:GLU:HA | 1 | 0.11 |
| (1,713) | 1:A:10:LEU:HD23 | 1:A:35:GLU:HA | 1 | 0.11 |
| (1,713) | 1:A:10:LEU:HD21 | 1:A:35:GLU:HA | 6 | 0.11 |
| (1,713) | 1:A:10:LEU:HD22 | 1:A:35:GLU:HA | 6 | 0.11 |
| (1,713) | 1:A:10:LEU:HD23 | 1:A:35:GLU:HA | 6 | 0.11 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG21 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG22 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG23 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG21 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG22 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG23 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG21 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG22 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG23 | 3 | 0.11 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG21 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG22 | 7 | 0.11 |
| (1,701) | 1:A:79:LEU:HD11 | 1:A:81:VAL:HG23 | 7 | 0.11 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG21 | 7 | 0.11 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG22 | 7 | 0.11 |
| (1,701) | 1:A:79:LEU:HD12 | 1:A:81:VAL:HG23 | 7 | 0.11 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG21 | 7 | 0.11 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG22 | 7 | 0.11 |
| (1,701) | 1:A:79:LEU:HD13 | 1:A:81:VAL:HG23 | 7 | 0.11 |
| (1,689) | 1:A:14:LEU:HG | 1:A:15:SER:H | 5 | 0.11 |
| (1,682) | 1:A:47:ARG:HG3 | 1:A:48:HIS:H | 6 | 0.11 |
| (1,682) | 1:A:47:ARG:HG3 | 1:A:48:HIS:H | 9 | 0.11 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE1 | 2 | 0.11 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE2 | 2 | 0.11 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE1 | 7 | 0.11 |
| (1,667) | 1:A:61:ARG:HG3 | 1:A:64:PHE:HE2 | 7 | 0.11 |
| (1,666) | 1:A:81:VAL:HG21 | 1:A:87:LEU:HG | 7 | 0.11 |
| (1,666) | 1:A:81:VAL:HG22 | 1:A:87:LEU:HG | 7 | 0.11 |
| (1,666) | 1:A:81:VAL:HG23 | 1:A:87:LEU:HG | 7 | 0.11 |
| (1,651) | 1:A:46:ILE:HG12 | 1:A:47:ARG:H | 9 | 0.11 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG2 | 4 | 0.11 |
| (1,647) | 1:A:99:GLU:HA | 1:A:103:PRO:HG3 | 4 | 0.11 |
| (1,633) | 1:A:37:TYR:HA | 1:A:40:ARG:HB2 | 9 | 0.11 |
| (1,622) | 1:A:3:ARG:HB3 | 1:A:4:THR:HA | 8 | 0.11 |
| (1,620) | 1:A:103:PRO:HB3 | 1:A:104:GLN:H | 7 | 0.11 |
| (1,58) | 1:A:82:LYS:H | 1:A:82:LYS:HD2 | 3 | 0.11 |
| (1,577) | 1:A:13:ARG:HB3 | 1:A:86:ARG:HD2 | 5 | 0.11 |
| (1,577) | 1:A:13:ARG:HB3 | 1:A:86:ARG:HD3 | 5 | 0.11 |
| (1,569) | 1:A:27:ILE:HB | 1:A:30:GLN:HE22 | 10 | 0.11 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG11 | 5 | 0.11 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG12 | 5 | 0.11 |
| (1,566) | 1:A:99:GLU:HG2 | 1:A:100:VAL:HG13 | 5 | 0.11 |
| (1,559) | 1:A:44:GLU:HG3 | 1:A:45:ASN:HA | 7 | 0.11 |
| (1,559) | 1:A:44:GLU:HG3 | 1:A:45:ASN:HA | 10 | 0.11 |
| (1,54) | 1:A:119:ASN:HA | 1:A:120:ASN:H | 1 | 0.11 |
| (1,54) | 1:A:119:ASN:HA | 1:A:120:ASN:H | 5 | 0.11 |
| (1,533) | 1:A:38:ALA:HA | 1:A:43:PHE:HB3 | 7 | 0.11 |
| (1,494) | 1:A:31:LYS:HE3 | 1:A:48:HIS:HB2 | 2 | 0.11 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG11 | 1 | 0.11 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG12 | 1 | 0.11 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG13 | 1 | 0.11 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG21 | 1 | 0.11 |
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG22 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,454) | 1:A:88:GLY:HA2 | 1:A:94:VAL:HG23 | 1 | 0.11 |
| (1,438) | 1:A:14:LEU:HB3 | 1:A:30:GLN:H | 6 | 0.11 |
| (1,428) | 1:A:102:PHE:HD1 | 1:A:103:PRO:HD2 | 6 | 0.11 |
| (1,428) | 1:A:102:PHE:HD2 | 1:A:103:PRO:HD2 | 6 | 0.11 |
| (1,406) | 1:A:41:ASN:HA | 1:A:42:GLY:H | 1 | 0.11 |
| (1,406) | 1:A:41:ASN:HA | 1:A:42:GLY:H | 4 | 0.11 |
| (1,406) | 1:A:41:ASN:HA | 1:A:42:GLY:H | 9 | 0.11 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE1 | 7 | 0.11 |
| (1,386) | 1:A:38:ALA:HA | 1:A:43:PHE:HE2 | 7 | 0.11 |
| (1,293) | 1:A:12:GLU:H | 1:A:50:THR:HA | 10 | 0.11 |
| (1,262) | 1:A:28:THR:HB | 1:A:29:ASN:H | 3 | 0.11 |
| (1,256) | 1:A:83:ASP:H | 1:A:86:ARG:HG3 | 5 | 0.11 |
| (1,250) | 1:A:13:ARG:HH11 | 1:A:86:ARG:HG2 | 2 | 0.11 |
| (1,250) | 1:A:13:ARG:HH11 | 1:A:86:ARG:HG2 | 6 | 0.11 |
| (1,229) | 1:A:39:ARG:HG2 | 1:A:41:ASN:H | 5 | 0.11 |
| (1,227) | 1:A:27:ILE:HD11 | 1:A:53:GLY:H | 2 | 0.11 |
| (1,227) | 1:A:27:ILE:HD12 | 1:A:53:GLY:H | 2 | 0.11 |
| (1,227) | 1:A:27:ILE:HD13 | 1:A:53:GLY:H | 2 | 0.11 |
| (1,222) | 1:A:83:ASP:HA | 1:A:85:SER:H | 9 | 0.11 |
| (1,1928) | 1:A:107:VAL:HG21 | 1:A:109:PHE:HB3 | 1 | 0.11 |
| (1,1928) | 1:A:107:VAL:HG22 | 1:A:109:PHE:HB3 | 1 | 0.11 |
| (1,1928) | 1:A:107:VAL:HG23 | 1:A:109:PHE:HB3 | 1 | 0.11 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD11 | 7 | 0.11 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD12 | 7 | 0.11 |
| (1,1904) | 1:A:47:ARG:HA | 1:A:7:ILE:HD13 | 7 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD11 | 1:A:18:ASP:HB2 | 9 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD12 | 1:A:18:ASP:HB2 | 9 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD13 | 1:A:18:ASP:HB2 | 9 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD21 | 1:A:18:ASP:HB2 | 9 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD22 | 1:A:18:ASP:HB2 | 9 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD23 | 1:A:18:ASP:HB2 | 9 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD11 | 1:A:18:ASP:HB2 | 10 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD12 | 1:A:18:ASP:HB2 | 10 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD13 | 1:A:18:ASP:HB2 | 10 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD21 | 1:A:18:ASP:HB2 | 10 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD22 | 1:A:18:ASP:HB2 | 10 | 0.11 |
| (1,1901) | 1:A:14:LEU:HD23 | 1:A:18:ASP:HB2 | 10 | 0.11 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 1 | 0.11 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 1 | 0.11 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 1 | 0.11 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 6 | 0.11 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 6 | 0.11 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG21 | 7 | 0.11 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG22 | 7 | 0.11 |
| (1,1895) | 1:A:28:THR:HA | 1:A:28:THR:HG23 | 7 | 0.11 |
| (1,1870) | 1:A:44:GLU:HA | 1:A:44:GLU:HG2 | 1 | 0.11 |
| (1,1870) | 1:A:44:GLU:HA | 1:A:44:GLU:HG2 | 4 | 0.11 |
| (1,1870) | 1:A:44:GLU:HA | 1:A:44:GLU:HG2 | 8 | 0.11 |
| (1,1870) | 1:A:44:GLU:HA | 1:A:44:GLU:HG2 | 9 | 0.11 |
| (1,1870) | 1:A:44:GLU:HA | 1:A:44:GLU:HG2 | 10 | 0.11 |
| (1,1869) | 1:A:57:VAL:HB | 1:A:58:ASN:HD22 | 9 | 0.11 |
| (1,1853) | 1:A:47:ARG:HA | 1:A:47:ARG:HD2 | 9 | 0.11 |
| (1,1853) | 1:A:47:ARG:HA | 1:A:47:ARG:HD3 | 9 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG11 | 4 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG12 | 4 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG13 | 4 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG21 | 4 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG22 | 4 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG23 | 4 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG11 | 6 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG12 | 6 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG13 | 6 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG21 | 6 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG22 | 6 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG23 | 6 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG11 | 8 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG12 | 8 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG13 | 8 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG21 | 8 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG22 | 8 | 0.11 |
| (1,1838) | 1:A:71:VAL:HA | 1:A:76:VAL:HG23 | 8 | 0.11 |
| (1,1837) | 1:A:28:THR:HA | 1:A:31:LYS:HD2 | 2 | 0.11 |
| (1,1837) | 1:A:28:THR:HA | 1:A:31:LYS:HD2 | 6 | 0.11 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD11 | 10 | 0.11 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD12 | 10 | 0.11 |
| (1,1831) | 1:A:37:TYR:HA | 1:A:112:ILE:HD13 | 10 | 0.11 |
| (1,1830) | 1:A:72:GLU:HA | 1:A:72:GLU:HG2 | 4 | 0.11 |
| (1,1823) | 1:A:32:LYS:HA | 1:A:32:LYS:HG2 | 6 | 0.11 |
| (1,1816) | 1:A:69:LYS:HA | 1:A:69:LYS:HG2 | 8 | 0.11 |
| (1,1807) | 1:A:23:GLU:HA | 1:A:23:GLU:HG2 | 10 | 0.11 |
| (1,1807) | 1:A:23:GLU:HA | 1:A:23:GLU:HG3 | 10 | 0.11 |
| (1,1789) | 1:A:78:THR:HA | 1:A:108:ARG:HA | 3 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 1 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 4 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 4 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 5 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 5 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 9 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 9 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD1 | 1:A:109:PHE:HA | 10 | 0.11 |
| (1,1788) | 1:A:102:PHE:HD2 | 1:A:109:PHE:HA | 10 | 0.11 |
| (1,1786) | 1:A:54:PHE:HZ | 1:A:62:PRO:HG3 | 8 | 0.11 |
| (1,1765) | 1:A:30:GLN:HE22 | 1:A:31:LYS:HA | 4 | 0.11 |
| (1,176) | 1:A:66:SER:H | 1:A:67:LEU:HB2 | 5 | 0.11 |
| (1,176) | 1:A:66:SER:H | 1:A:67:LEU:HB2 | 10 | 0.11 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 2 | 0.11 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 2 | 0.11 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD1 | 5 | 0.11 |
| (1,1754) | 1:A:13:ARG:HB3 | 1:A:54:PHE:HD2 | 5 | 0.11 |
| (1,1748) | 1:A:54:PHE:HE1 | 1:A:62:PRO:HG2 | 5 | 0.11 |
| (1,1748) | 1:A:54:PHE:HE2 | 1:A:62:PRO:HG2 | 5 | 0.11 |
| (1,1720) | 1:A:33:TYR:HD1 | 1:A:34:LEU:HD11 | 10 | 0.11 |
| (1,1720) | 1:A:33:TYR:HD1 | 1:A:34:LEU:HD12 | 10 | 0.11 |
| (1,1720) | 1:A:33:TYR:HD1 | 1:A:34:LEU:HD13 | 10 | 0.11 |
| (1,1720) | 1:A:33:TYR:HD2 | 1:A:34:LEU:HD11 | 10 | 0.11 |
| (1,1720) | 1:A:33:TYR:HD2 | 1:A:34:LEU:HD12 | 10 | 0.11 |
| (1,1720) | 1:A:33:TYR:HD2 | 1:A:34:LEU:HD13 | 10 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD1 | 1 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD2 | 1 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD1 | 1 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD2 | 1 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD1 | 1 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD2 | 1 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD1 | 6 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD21 | 1:A:49:PHE:HD2 | 6 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD1 | 6 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD22 | 1:A:49:PHE:HD2 | 6 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD1 | 6 | 0.11 |
| (1,1715) | 1:A:10:LEU:HD23 | 1:A:49:PHE:HD2 | 6 | 0.11 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD11 | 9 | 0.11 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD12 | 9 | 0.11 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD13 | 9 | 0.11 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD11 | 10 | 0.11 |
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD12 | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1707) | 1:A:67:LEU:H | 1:A:67:LEU:HD13 | 10 | 0.11 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD11 | 9 | 0.11 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD12 | 9 | 0.11 |
| (1,1703) | 1:A:64:PHE:HA | 1:A:67:LEU:HD13 | 9 | 0.11 |
| (1,168) | 1:A:103:PRO:HD3 | 1:A:104:GLN:H | 2 | 0.11 |
| (1,168) | 1:A:103:PRO:HD3 | 1:A:104:GLN:H | 7 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD21 | 9 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD22 | 9 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD21 | 1:A:34:LEU:HD23 | 9 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD21 | 9 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD22 | 9 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD22 | 1:A:34:LEU:HD23 | 9 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD21 | 9 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD22 | 9 | 0.11 |
| (1,1639) | 1:A:10:LEU:HD23 | 1:A:34:LEU:HD23 | 9 | 0.11 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD21 | 9 | 0.11 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD22 | 9 | 0.11 |
| (1,1632) | 1:A:10:LEU:HA | 1:A:10:LEU:HD23 | 9 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG21 | 1:A:102:PHE:HD1 | 2 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG21 | 1:A:102:PHE:HD2 | 2 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG22 | 1:A:102:PHE:HD1 | 2 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG22 | 1:A:102:PHE:HD2 | 2 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG23 | 1:A:102:PHE:HD1 | 2 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG23 | 1:A:102:PHE:HD2 | 2 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG21 | 1:A:102:PHE:HD1 | 7 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG21 | 1:A:102:PHE:HD2 | 7 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG22 | 1:A:102:PHE:HD1 | 7 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG22 | 1:A:102:PHE:HD2 | 7 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG23 | 1:A:102:PHE:HD1 | 7 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG23 | 1:A:102:PHE:HD2 | 7 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG21 | 1:A:102:PHE:HD1 | 9 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG21 | 1:A:102:PHE:HD2 | 9 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG22 | 1:A:102:PHE:HD1 | 9 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG22 | 1:A:102:PHE:HD2 | 9 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG23 | 1:A:102:PHE:HD1 | 9 | 0.11 |
| (1,1620) | 1:A:71:VAL:HG23 | 1:A:102:PHE:HD2 | 9 | 0.11 |
| (1,161) | 1:A:10:LEU:HD11 | 1:A:46:ILE:H | 6 | 0.11 |
| (1,161) | 1:A:10:LEU:HD12 | 1:A:46:ILE:H | 6 | 0.11 |
| (1,161) | 1:A:10:LEU:HD13 | 1:A:46:ILE:H | 6 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD11 | 1:A:93:GLN:HB2 | 1 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD11 | 1:A:93:GLN:HB3 | 1 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD12 | 1:A:93:GLN:HB2 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1577) | 1:A:92:LEU:HD12 | 1:A:93:GLN:HB3 | 1 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD13 | 1:A:93:GLN:HB2 | 1 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD13 | 1:A:93:GLN:HB3 | 1 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD11 | 1:A:93:GLN:HB2 | 2 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD11 | 1:A:93:GLN:HB3 | 2 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD12 | 1:A:93:GLN:HB2 | 2 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD12 | 1:A:93:GLN:HB3 | 2 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD13 | 1:A:93:GLN:HB2 | 2 | 0.11 |
| (1,1577) | 1:A:92:LEU:HD13 | 1:A:93:GLN:HB3 | 2 | 0.11 |
| (1,1563) | 1:A:68:ILE:HG21 | 1:A:72:GLU:HG3 | 7 | 0.11 |
| (1,1563) | 1:A:68:ILE:HG22 | 1:A:72:GLU:HG3 | 7 | 0.11 |
| (1,1563) | 1:A:68:ILE:HG23 | 1:A:72:GLU:HG3 | 7 | 0.11 |
| (1,1563) | 1:A:68:ILE:HG21 | 1:A:72:GLU:HG3 | 8 | 0.11 |
| (1,1563) | 1:A:68:ILE:HG22 | 1:A:72:GLU:HG3 | 8 | 0.11 |
| (1,1563) | 1:A:68:ILE:HG23 | 1:A:72:GLU:HG3 | 8 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG21 | 2 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG22 | 2 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG23 | 2 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG21 | 3 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG22 | 3 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG23 | 3 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG21 | 6 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG22 | 6 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG23 | 6 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG21 | 7 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG22 | 7 | 0.11 |
| (1,1535) | 1:A:116:ILE:HA | 1:A:116:ILE:HG23 | 7 | 0.11 |
| (1,1534) | 1:A:57:VAL:HG11 | 1:A:58:ASN:HD22 | 9 | 0.11 |
| (1,1534) | 1:A:57:VAL:HG12 | 1:A:58:ASN:HD22 | 9 | 0.11 |
| (1,1534) | 1:A:57:VAL:HG13 | 1:A:58:ASN:HD22 | 9 | 0.11 |
| (1,1534) | 1:A:57:VAL:HG21 | 1:A:58:ASN:HD22 | 9 | 0.11 |
| (1,1534) | 1:A:57:VAL:HG22 | 1:A:58:ASN:HD22 | 9 | 0.11 |
| (1,1534) | 1:A:57:VAL:HG23 | 1:A:58:ASN:HD22 | 9 | 0.11 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD11 | 2 | 0.11 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD12 | 2 | 0.11 |
| (1,1509) | 1:A:77:GLU:H | 1:A:7:ILE:HD13 | 2 | 0.11 |
| (1,1507) | 1:A:96:PHE:HD1 | 1:A:101:LEU:HG | 2 | 0.11 |
| (1,1507) | 1:A:96:PHE:HD2 | 1:A:101:LEU:HG | 2 | 0.11 |
| (1,1507) | 1:A:96:PHE:HD1 | 1:A:101:LEU:HG | 9 | 0.11 |
| (1,1507) | 1:A:96:PHE:HD2 | 1:A:101:LEU:HG | 9 | 0.11 |
| (1,1507) | 1:A:96:PHE:HD1 | 1:A:101:LEU:HG | 10 | 0.11 |
| (1,1507) | 1:A:96:PHE:HD2 | 1:A:101:LEU:HG | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 2 | 0.11 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 2 | 0.11 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 2 | 0.11 |
| (1,1506) | 1:A:68:ILE:HD11 | 1:A:101:LEU:HG | 9 | 0.11 |
| (1,1506) | 1:A:68:ILE:HD12 | 1:A:101:LEU:HG | 9 | 0.11 |
| (1,1506) | 1:A:68:ILE:HD13 | 1:A:101:LEU:HG | 9 | 0.11 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG21 | 5 | 0.11 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG22 | 5 | 0.11 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG23 | 5 | 0.11 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG21 | 6 | 0.11 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG22 | 6 | 0.11 |
| (1,1474) | 1:A:11:TYR:HA | 1:A:81:VAL:HG23 | 6 | 0.11 |
| (1,1470) | 1:A:74:GLY:HA3 | 1:A:105:LYS:HG2 | 2 | 0.11 |
| (1,1470) | 1:A:74:GLY:HA3 | 1:A:105:LYS:HG2 | 4 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB1 | 1 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB2 | 1 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB3 | 1 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB1 | 5 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB2 | 5 | 0.11 |
| (1,1466) | 1:A:72:GLU:H | 1:A:73:ALA:HB3 | 5 | 0.11 |
| (1,1446) | 1:A:66:SER:HA | 1:A:69:LYS:HD2 | 10 | 0.11 |
| (1,1446) | 1:A:66:SER:HA | 1:A:69:LYS:HD3 | 10 | 0.11 |
| (1,1440) | 1:A:6:ARG:HG3 | 1:A:75:ASN:HA | 1 | 0.11 |
| (1,1440) | 1:A:6:ARG:HG3 | 1:A:75:ASN:HA | 2 | 0.11 |
| (1,1440) | 1:A:6:ARG:HG3 | 1:A:75:ASN:HA | 10 | 0.11 |
| (1,1432) | 1:A:34:LEU:H | 1:A:34:LEU:HB3 | 4 | 0.11 |
| (1,1423) | 1:A:13:ARG:HB3 | 1:A:13:ARG:HH12 | 10 | 0.11 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 3 | 0.11 |
| (1,1419) | 1:A:44:GLU:HG2 | 1:A:45:ASN:HD21 | 4 | 0.11 |
| (1,1402) | 1:A:37:TYR:HE1 | 1:A:41:ASN:HB3 | 6 | 0.11 |
| (1,1402) | 1:A:37:TYR:HE2 | 1:A:41:ASN:HB3 | 6 | 0.11 |
| (1,1399) | 1:A:70:GLU:HA | 1:A:72:GLU:HG3 | 8 | 0.11 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG21 | 9 | 0.11 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG22 | 9 | 0.11 |
| (1,1398) | 1:A:11:TYR:HB2 | 1:A:81:VAL:HG23 | 9 | 0.11 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD11 | 7 | 0.11 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD12 | 7 | 0.11 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD13 | 7 | 0.11 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD21 | 7 | 0.11 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD22 | 7 | 0.11 |
| (1,1395) | 1:A:18:ASP:HB2 | 1:A:20:LEU:HD23 | 7 | 0.11 |
| (1,1383) | 1:A:103:PRO:HA | 1:A:106:ASN:HB2 | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1383) | 1:A:103:PRO:HA | 1:A:106:ASN:HB2 | 8 | 0.11 |
| (1,1358) | 1:A:6:ARG:HE | 1:A:45:ASN:HB2 | 2 | 0.11 |
| (1,1358) | 1:A:6:ARG:HE | 1:A:45:ASN:HB3 | 2 | 0.11 |
| (1,1342) | 1:A:6:ARG:HA | 1:A:75:ASN:HB3 | 3 | 0.11 |
| (1,1340) | 1:A:7:ILE:HB | 1:A:75:ASN:HB3 | 4 | 0.11 |
| (1,1334) | 1:A:111:ALA:H | 1:A:112:ILE:HA | 1 | 0.11 |
| (1,1334) | 1:A:111:ALA:H | 1:A:112:ILE:HA | 2 | 0.11 |
| (1,1323) | 1:A:71:VAL:HA | 1:A:105:LYS:HG2 | 9 | 0.11 |
| (1,1307) | 1:A:5:SER:H | 1:A:5:SER:HB2 | 9 | 0.11 |
| (1,1307) | 1:A:5:SER:H | 1:A:5:SER:HB3 | 9 | 0.11 |
| (1,1263) | 1:A:21:THR:HA | 1:A:21:THR:HB | 3 | 0.11 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 2 | 0.11 |
| (1,1249) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HA | 8 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 2 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 3 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 4 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 5 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 6 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 7 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 8 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 9 | 0.11 |
| (1,1247) | 1:A:108:ARG:HA | 1:A:109:PHE:HA | 10 | 0.11 |
| (1,1244) | 1:A:47:ARG:HA | 1:A:48:HIS:HA | 5 | 0.11 |
| (1,1234) | 1:A:64:PHE:HZ | 1:A:68:ILE:HG12 | 7 | 0.11 |
| (1,1234) | 1:A:64:PHE:HZ | 1:A:68:ILE:HG13 | 7 | 0.11 |
| (1,1222) | 1:A:93:GLN:HA | 1:A:96:PHE:HD1 | 3 | 0.11 |
| (1,1222) | 1:A:93:GLN:HA | 1:A:96:PHE:HD2 | 3 | 0.11 |
| (1,1201) | 1:A:59:PHE:HB3 | 1:A:64:PHE:HD1 | 2 | 0.11 |
| (1,1201) | 1:A:59:PHE:HB3 | 1:A:64:PHE:HD2 | 2 | 0.11 |
| (1,1196) | 1:A:60:ASN:HD22 | 1:A:64:PHE:HE1 | 3 | 0.11 |
| (1,1196) | 1:A:60:ASN:HD22 | 1:A:64:PHE:HE2 | 3 | 0.11 |
| (1,119) | 1:A:44:GLU:H | 1:A:46:ILE:H | 8 | 0.11 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 4 | 0.11 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 4 | 0.11 |
| (1,1167) | 1:A:91:TYR:HE1 | 1:A:117:ASP:HA | 9 | 0.11 |
| (1,1167) | 1:A:91:TYR:HE2 | 1:A:117:ASP:HA | 9 | 0.11 |
| (1,1116) | 1:A:5:SER:HA | 1:A:45:ASN:HD22 | 9 | 0.11 |
| (1,1109) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HE1 | 6 | 0.11 |
| (1,1109) | 1:A:79:LEU:HB2 | 1:A:109:PHE:HE2 | 6 | 0.11 |
| (1,110) | 1:A:19:ASP:HA | 1:A:20:LEU:H | 2 | 0.11 |
| (1,110) | 1:A:19:ASP:HA | 1:A:20:LEU:H | 7 | 0.11 |
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD11 | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD12 | 10 | 0.11 |
| (1,1077) | 1:A:49:PHE:HD1 | 1:A:67:LEU:HD13 | 10 | 0.11 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD11 | 10 | 0.11 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD12 | 10 | 0.11 |
| (1,1077) | 1:A:49:PHE:HD2 | 1:A:67:LEU:HD13 | 10 | 0.11 |
| (1,1053) | 1:A:81:VAL:HG21 | 1:A:87:LEU:H | 9 | 0.11 |
| (1,1053) | 1:A:81:VAL:HG22 | 1:A:87:LEU:H | 9 | 0.11 |
| (1,1053) | 1:A:81:VAL:HG23 | 1:A:87:LEU:H | 9 | 0.11 |
| (1,1011) | 1:A:32:LYS:H | 1:A:48:HIS:HE1 | 7 | 0.11 |
| (1,1008) | 1:A:112:ILE:H | 1:A:112:ILE:HG12 | 7 | 0.11 |
| (1,1003) | 1:A:75:ASN:H | 1:A:75:ASN:HB3 | 1 | 0.11 |

# 10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found