# Full wwPDB NMR Structure Validation Report (i)

Nov 7, 2023 – 03:55 PM EST

| | | |
|---|---|---|
| PDB ID | : | 2K05 |
| BMRB ID | : | 15637 |
| Title | : | Structure of SDF1 in complex with the CXCR4 N-terminus containing sulfotyrosines at postitions 7, 12 and 21 |
| Authors | : | Volkman, B.F.; Veldkamp, C.T.; Peterson, F.C. |
| Deposited on | : | 2008-01-24 |

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

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

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

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

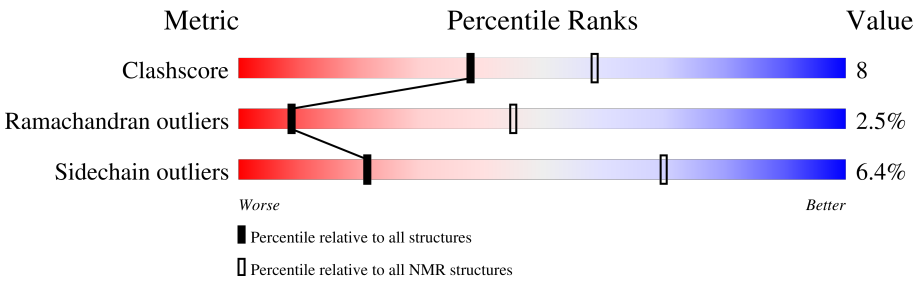
| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | 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) | : | 2.36 |

# 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 88%.

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 | 70 | 69% 13% 16% . |
| 1 | C | 70 | 61% 19% 17% . |
| 2 | B | 40 | 20% 75% 5% |
| 2 | D | 40 | 20% 75% 5% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:8-A:43, A:47-A:67, B:119-B:120, B:122-B:127, C:209-C:243, C:247-C:267, D:319-D:320, D:322-D:327 (129) | 0.94 | 13 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

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

# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3429 atoms, of which 1682 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Stromal cell-derived factor 1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 68 | 1136 | 353 | 579 | 106 | 92 | 6 | 0 |
| 1 | C | 68 | 1136 | 353 | 579 | 106 | 92 | 6 | 0 |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -1 | GLY | - | expression tag | UNP P48061 |
| A | 0 | MET | - | expression tag | UNP P48061 |
| A | 36 | CYS | LEU | engineered mutation | UNP P48061 |
| A | 65 | CYS | ALA | engineered mutation | UNP P48061 |
| C | 199 | GLY | - | expression tag | UNP P48061 |
| C | 200 | MET | - | expression tag | UNP P48061 |
| C | 236 | CYS | LEU | engineered mutation | UNP P48061 |
| C | 265 | CYS | ALA | engineered mutation | UNP P48061 |

- Molecule 2 is a protein called C-X-C chemokine receptor type 4.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 2 | B | 38 | 578 | 185 | 262 | 47 | 78 | 6 | 0 |
| 2 | D | 38 | 579 | 185 | 262 | 47 | 79 | 6 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 99 | GLY | - | expression tag | UNP P61073 |
| B | 100 | SER | - | expression tag | UNP P61073 |
| B | 128 | ALA | CYS | engineered mutation | UNP P61073 |
| D | 299 | GLY | - | expression tag | UNP P61073 |
| D | 300 | SER | - | expression tag | UNP P61073 |
| D | 328 | ALA | CYS | engineered mutation | UNP P61073 |

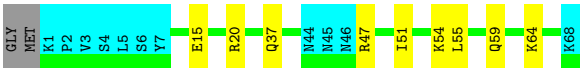
# 4 Residue-property plots (i)

## 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: Stromal cell-derived factor 1

Chain A:

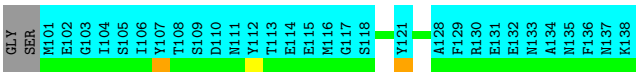



• Molecule 1: Stromal cell-derived factor 1

Chain C:

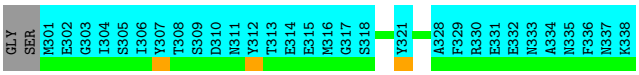
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:




• Molecule 2: C-X-C chemokine receptor type 4

Chain D:



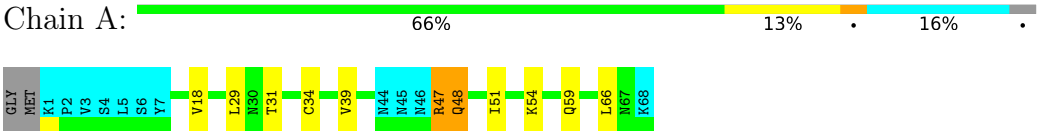

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

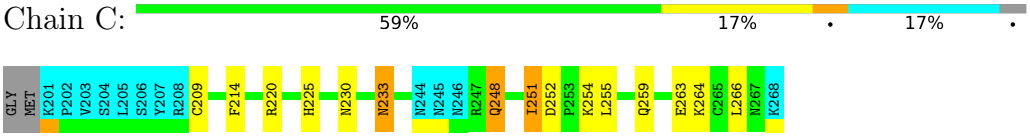
- Molecule 1: Stromal cell-derived factor 1

Chain A:



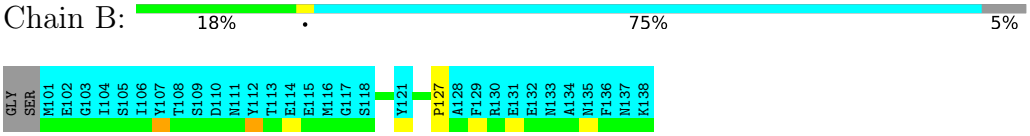

- Molecule 1: Stromal cell-derived factor 1

Chain C:



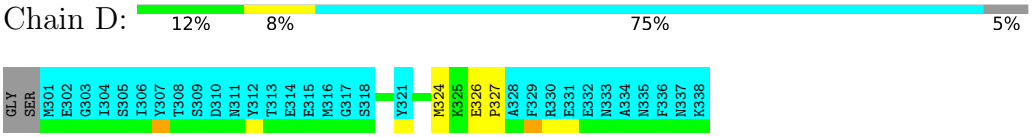

- Molecule 2: C-X-C chemokine receptor type 4

Chain B:




- Molecule 2: C-X-C chemokine receptor type 4

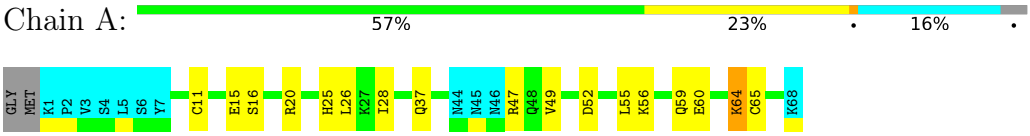
Chain D:




### 4.2.2 Score per residue for model 2

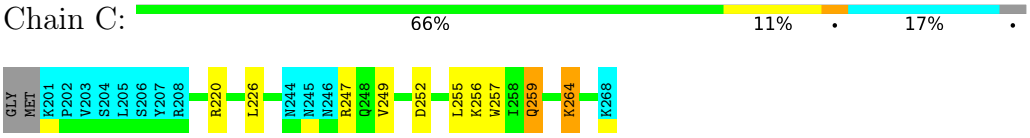
- Molecule 1: Stromal cell-derived factor 1

Chain A:




- Molecule 1: Stromal cell-derived factor 1

Chain C:

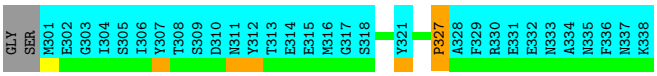



- Molecule 2: C-X-C chemokine receptor type 4

Chain B:

• Molecule 2: C-X-C chemokine receptor type 4

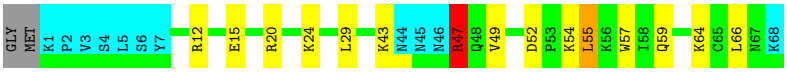
Chain D:




### 4.2.3 Score per residue for model 3

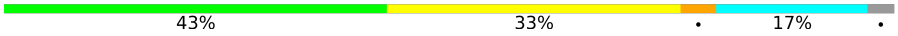
• Molecule 1: Stromal cell-derived factor 1

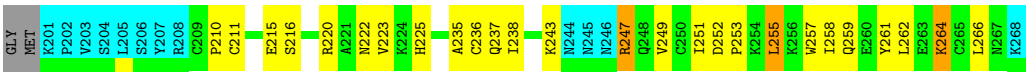
Chain A:




• Molecule 1: Stromal cell-derived factor 1

Chain C:



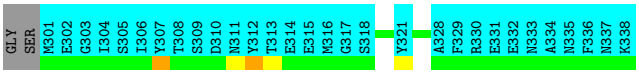




• Molecule 2: C-X-C chemokine receptor type 4

Chain B:

• Molecule 2: C-X-C chemokine receptor type 4

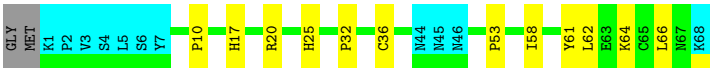
Chain D:




### 4.2.4 Score per residue for model 4

• Molecule 1: Stromal cell-derived factor 1

Chain A:



- Molecule 1: Stromal cell-derived factor 1

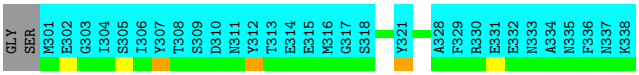
Chain C:

- Molecule 2: C-X-C chemokine receptor type 4

Chain B:

- Molecule 2: C-X-C chemokine receptor type 4

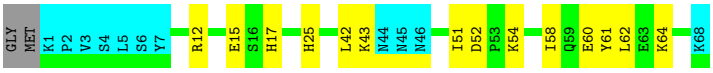
Chain D:




### 4.2.5 Score per residue for model 5

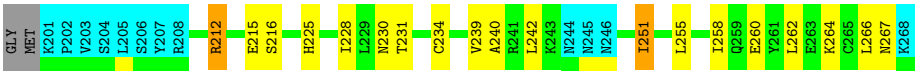
- Molecule 1: Stromal cell-derived factor 1

Chain A:



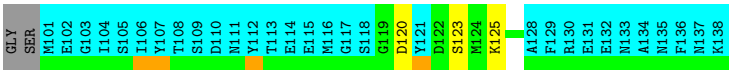

- Molecule 1: Stromal cell-derived factor 1

Chain C:



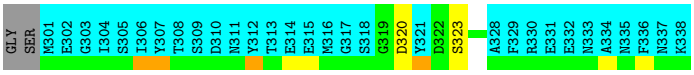

- Molecule 2: C-X-C chemokine receptor type 4

Chain B:




- Molecule 2: C-X-C chemokine receptor type 4

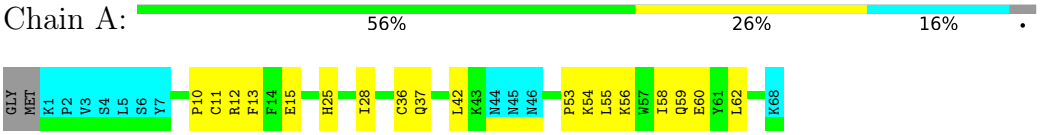
Chain D:



### 4.2.6 Score per residue for model 6

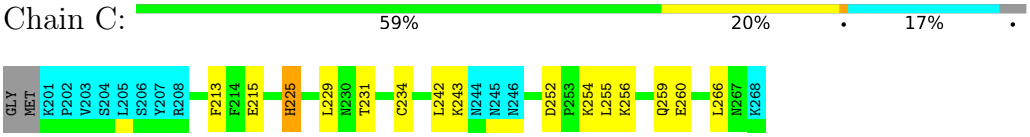
- Molecule 1: Stromal cell-derived factor 1

Chain A:



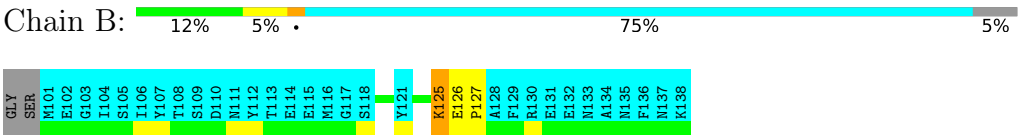

- Molecule 1: Stromal cell-derived factor 1

Chain C:



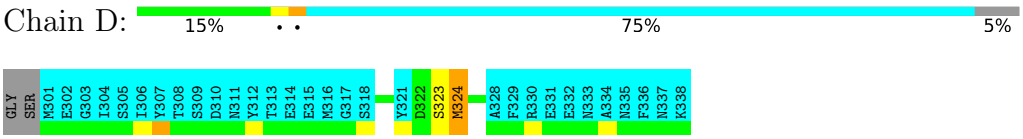

- Molecule 2: C-X-C chemokine receptor type 4

Chain B:




- Molecule 2: C-X-C chemokine receptor type 4

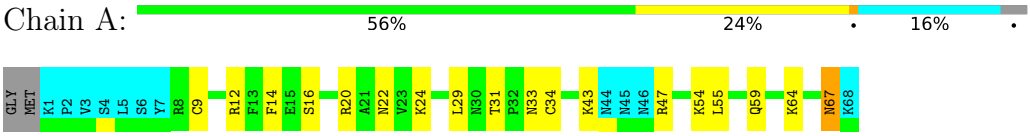
Chain D:




### 4.2.7 Score per residue for model 7

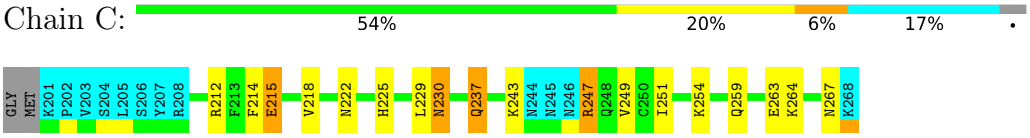
- Molecule 1: Stromal cell-derived factor 1

Chain A:



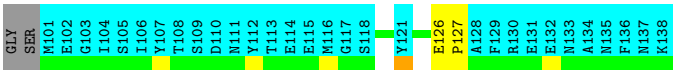

- Molecule 1: Stromal cell-derived factor 1

Chain C:



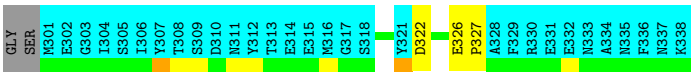

- Molecule 2: C-X-C chemokine receptor type 4

Chain B:




• Molecule 2: C-X-C chemokine receptor type 4

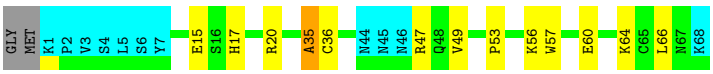
Chain D: 12% 8% 75% 5%




### 4.2.8 Score per residue for model 8

• Molecule 1: Stromal cell-derived factor 1

Chain A: 63% 17% • 16% •

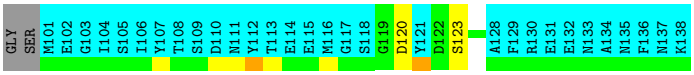



• Molecule 1: Stromal cell-derived factor 1

Chain C: 57% 23% 17% •

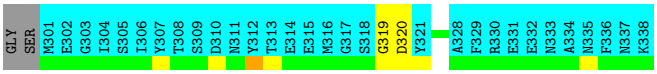
• Molecule 2: C-X-C chemokine receptor type 4

Chain B: 15% 5% 75% 5%




• Molecule 2: C-X-C chemokine receptor type 4

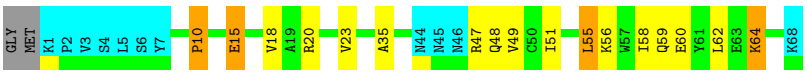
Chain D: 15% 5% 75% 5%




### 4.2.9 Score per residue for model 9

• Molecule 1: Stromal cell-derived factor 1

Chain A: 57% 19% 6% 16% •



• Molecule 1: Stromal cell-derived factor 1

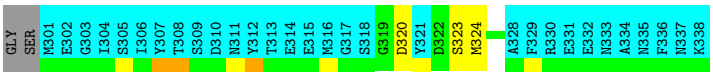
Chain C: 56% 21% 17%

• Molecule 2: C-X-C chemokine receptor type 4

Chain B: 20% 75% 5%

• Molecule 2: C-X-C chemokine receptor type 4

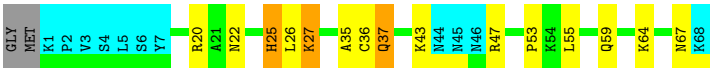
Chain D: 12% 8% 75% 5%




### 4.2.10 Score per residue for model 10

• Molecule 1: Stromal cell-derived factor 1

Chain A: 60% 17% 16%




• Molecule 1: Stromal cell-derived factor 1

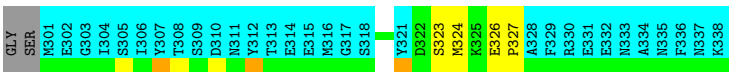
Chain C: 50% 20% 9% 17%

• Molecule 2: C-X-C chemokine receptor type 4

Chain B: 18% 75% 5%

• Molecule 2: C-X-C chemokine receptor type 4

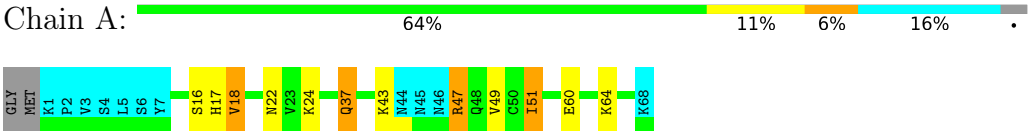
Chain D: 10% 10% 75% 5%



### 4.2.11 Score per residue for model 11

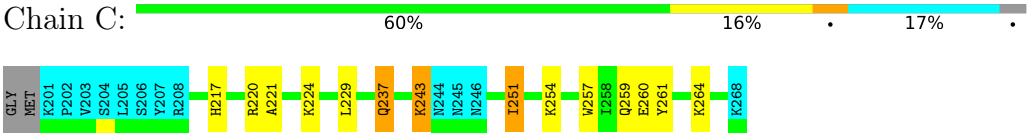
- Molecule 1: Stromal cell-derived factor 1

Chain A:



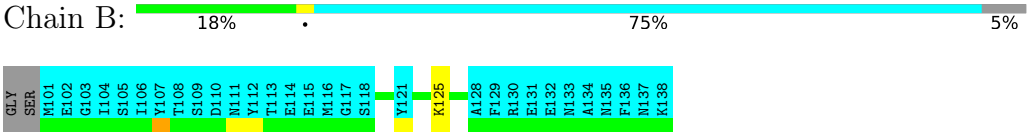

- Molecule 1: Stromal cell-derived factor 1

Chain C:



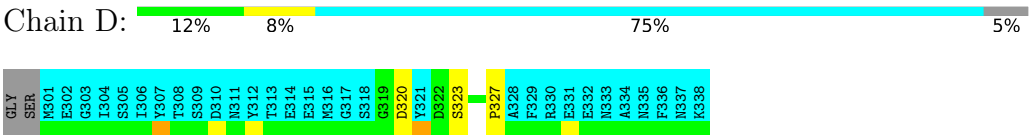

- Molecule 2: C-X-C chemokine receptor type 4

Chain B:




- Molecule 2: C-X-C chemokine receptor type 4

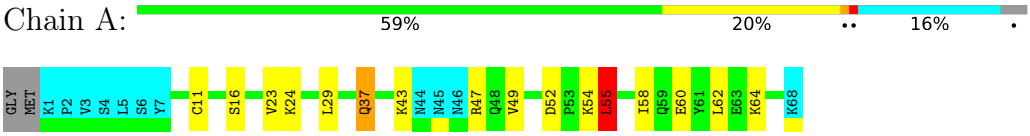
Chain D:




### 4.2.12 Score per residue for model 12

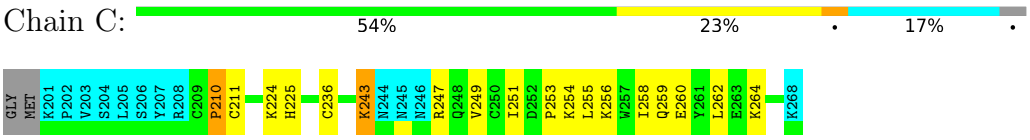
- Molecule 1: Stromal cell-derived factor 1

Chain A:



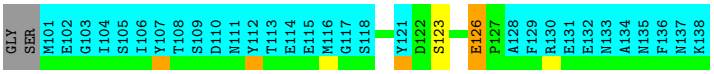

- Molecule 1: Stromal cell-derived factor 1

Chain C:




- Molecule 2: C-X-C chemokine receptor type 4

Chain B:



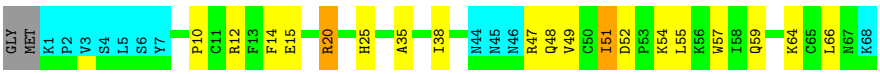

• Molecule 2: C-X-C chemokine receptor type 4

Chain D: 12% 8% 75% 5%

### 4.2.13 Score per residue for model 13 (medoid)

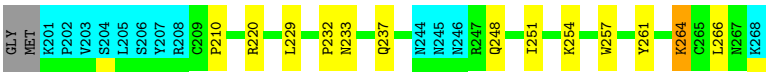
• Molecule 1: Stromal cell-derived factor 1

Chain A: 54% 24% • 16% •




• Molecule 1: Stromal cell-derived factor 1

Chain C: 61% 17% • 17% •

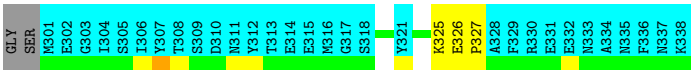



• Molecule 2: C-X-C chemokine receptor type 4

Chain B: 15% 5% 75% 5%

• Molecule 2: C-X-C chemokine receptor type 4

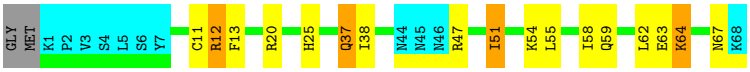
Chain D: 12% 8% 75% 5%




### 4.2.14 Score per residue for model 14

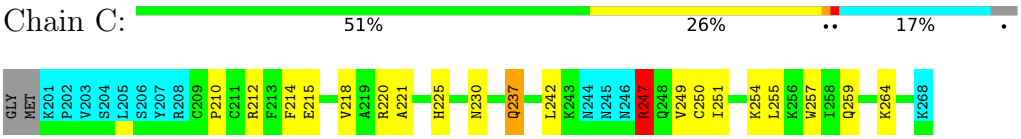
• Molecule 1: Stromal cell-derived factor 1

Chain A: 57% 19% 6% 16% •



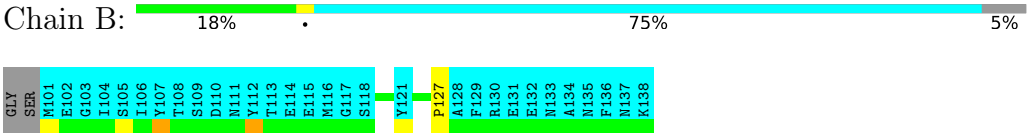
- Molecule 1: Stromal cell-derived factor 1

Chain C:



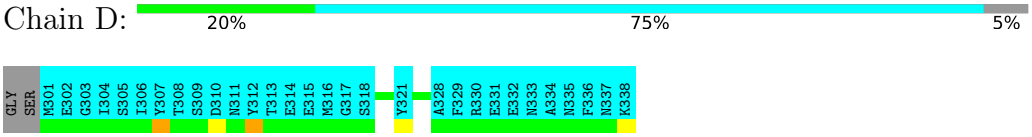

- Molecule 2: C-X-C chemokine receptor type 4

Chain B:




- Molecule 2: C-X-C chemokine receptor type 4

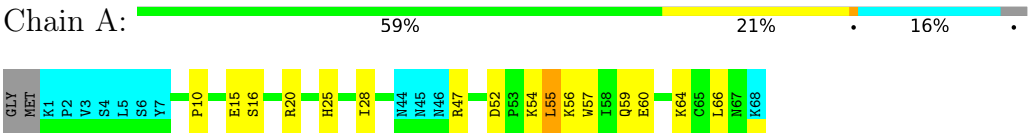
Chain D:




### 4.2.15 Score per residue for model 15

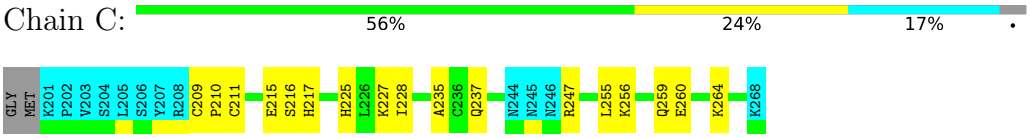
- Molecule 1: Stromal cell-derived factor 1

Chain A:



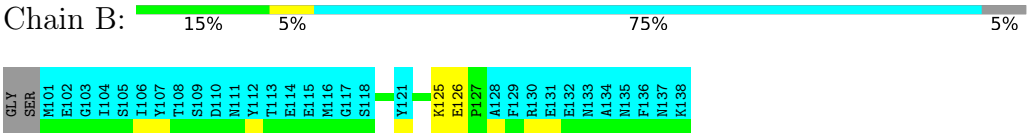

- Molecule 1: Stromal cell-derived factor 1

Chain C:



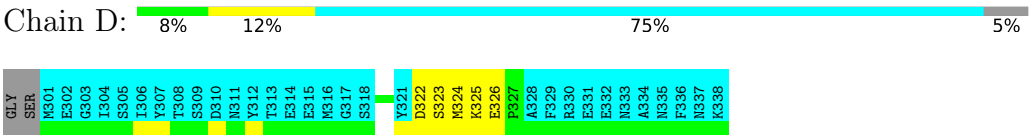

- Molecule 2: C-X-C chemokine receptor type 4

Chain B:




- Molecule 2: C-X-C chemokine receptor type 4

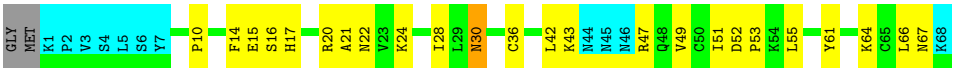
Chain D:



### 4.2.16 Score per residue for model 16

- Molecule 1: Stromal cell-derived factor 1

Chain A: 47% 33% • 16% •

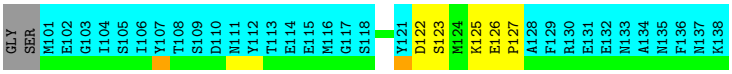



- Molecule 1: Stromal cell-derived factor 1

Chain C: 54% 21% • 17% •

- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 8% 12% 75% 5%



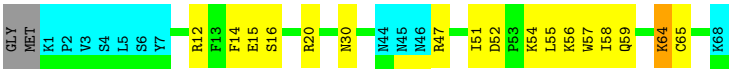

- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 12% 5% • 75% 5%

### 4.2.17 Score per residue for model 17

- Molecule 1: Stromal cell-derived factor 1

Chain A: 57% 23% • 16% •

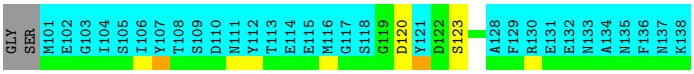



- Molecule 1: Stromal cell-derived factor 1

Chain C: 56% 23% • 17% •

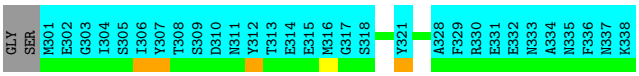
- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 15% 5% 75% 5%




• Molecule 2: C-X-C chemokine receptor type 4

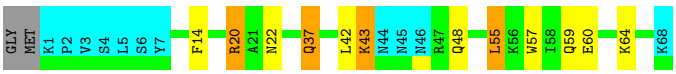
Chain D: 20% 75% 5%




### 4.2.18 Score per residue for model 18

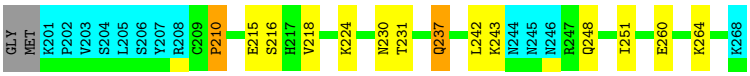
• Molecule 1: Stromal cell-derived factor 1

Chain A: 64% 11% 6% 16% •



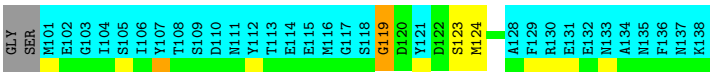

• Molecule 1: Stromal cell-derived factor 1

Chain C: 60% 17% • 17% •



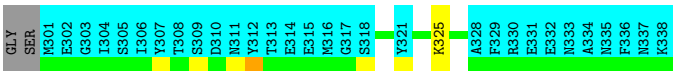

• Molecule 2: C-X-C chemokine receptor type 4

Chain B: 12% 5% • 75% 5%




• Molecule 2: C-X-C chemokine receptor type 4

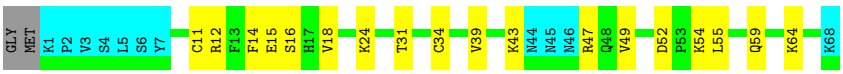
Chain D: 18% • 75% 5%




### 4.2.19 Score per residue for model 19

• Molecule 1: Stromal cell-derived factor 1

Chain A: 56% 26% 16% •



- Molecule 1: Stromal cell-derived factor 1

Chain C: 56% 23% • 17% •

GLY MET K201 P202 V203 S204 L205 S206 Y207 R208 C211 R212 F213 F214 E215 K224 K227 T231 C234 V239 K243 N244 N245 N246 C250 I251 D252 P253 K254 L255 Q259 E260 K264 K268

- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 8% 12% 75% 5%

GLY SER M101 E102 G103 I104 S105 I106 Y107 T108 S109 D110 N111 Y112 T113 E114 E115 M116 G117 S118 Y121 D122 S123 M124 K125 E126 P127 A128 F129 R130 E131 E132 N133 A134 N135 F136 N137 K138

- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 10% 10% 75% 5%

GLY SER M301 E302 G303 I304 S305 I306 Y307 T308 S309 D310 N311 Y312 T313 E314 E315 M316 G317 S318 G319 D320 Y321 D322 S323 M324 K325 E326 F327 A328 F329 R330 E331 E332 N333 A334 N335 F336 N337 K338

### 4.2.20 Score per residue for model 20

- Molecule 1: Stromal cell-derived factor 1

Chain A: 59% 21% • 16% •

GLY MET K1 P2 V3 S4 L5 S6 Y7 P10 C11 R12 F13 F14 R20 C36 Q37 I38 N44 N45 N46 I51 D52 P53 K54 L55 K56 Q59 E60 E63 K64 K68

- Molecule 1: Stromal cell-derived factor 1

Chain C: 59% 20% • 17% •

GLY MET K201 P202 V203 S204 L205 S206 Y207 R208 R212 E215 L229 C236 Q237 I238 V239 N244 N245 N246 I251 D252 P253 K254 L255 Q259 E260 K264 N267 K268

- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 15% 5% 75% 5%

GLY SER M101 E102 G103 I104 S105 I106 Y107 T108 S109 D110 N111 Y112 T113 E114 E115 M116 G117 S118 G119 D120 Y121 D122 S123 A128 F129 R130 E131 E132 N133 A134 N135 F136 N137 K138

- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 18% • 75% 5%

GLY SER M301 E302 G303 I304 S305 I306 Y307 T308 S309 D310 N311 Y312 T313 E314 E315 M316 G317 S318 Y321 K325 A328 F329 R330 E331 E332 N333 A334 N335 F336 N337 K338

# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT..*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

| **Software name** | **Classification** | **Version** |
|---|---|---|
| CYANA | structure solution | 2.1 |
| X-PLOR NIH | refinement | 2.9.3 |

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 | 2494 |
| Number of shifts mapped to atoms | 2494 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 88% |

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|---|---|---|---|
| 1 | C | 0.0±0.0 | 0.1±0.3 |
| 1 | A | 0.0±0.0 | 0.1±0.2 |
| All | All | 0 | 3 |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 1 | A | 47 | ARG | Sidechain | 1 |
| 1 | C | 220 | ARG | Sidechain | 1 |
| 1 | C | 247 | ARG | Sidechain | 1 |

## 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 | 469 | 489 | 487 | 9±2 |
| 1 | C | 458 | 476 | 474 | 9±3 |
| 2 | B | 59 | 51 | 51 | 1±1 |
| 2 | D | 59 | 51 | 51 | 1±1 |
| All | All | 20900 | 21340 | 21260 | 338 |

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 8.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:14:PHE:O | 2:B:123:SER:HA | 0.71 | 1.86 | 19 | 2 |
| 1:A:60:GLU:O | 1:A:64:LYS:HG2 | 0.66 | 1.91 | 18 | 7 |
| 1:C:220:ARG:HB3 | 1:C:257:TRP:CE3 | 0.64 | 2.28 | 11 | 6 |
| 1:A:20:ARG:HB3 | 1:A:57:TRP:CE3 | 0.63 | 2.28 | 17 | 4 |
| 1:C:260:GLU:O | 1:C:264:LYS:HG2 | 0.63 | 1.93 | 11 | 9 |
| 1:C:218:VAL:HG11 | 1:C:251:ILE:HD12 | 0.60 | 1.73 | 7 | 2 |
| 1:C:224:LYS:CG | 1:C:243:LYS:HA | 0.58 | 2.28 | 19 | 2 |
| 1:A:54:LYS:HA | 1:A:59:GLN:NE2 | 0.57 | 2.14 | 20 | 4 |
| 1:A:37:GLN:HE21 | 1:A:37:GLN:HA | 0.57 | 1.59 | 10 | 5 |
| 1:C:212:ARG:HA | 1:C:212:ARG:NE | 0.57 | 2.13 | 14 | 2 |
| 1:C:224:LYS:HE3 | 1:C:243:LYS:O | 0.56 | 2.00 | 18 | 1 |
| 1:A:54:LYS:O | 2:B:127:PRO:HA | 0.56 | 1.99 | 6 | 4 |
| 1:A:20:ARG:HG2 | 1:A:57:TRP:CE3 | 0.56 | 2.35 | 8 | 2 |
| 1:C:238:ILE:HB | 1:C:251:ILE:O | 0.56 | 1.99 | 3 | 1 |
| 1:C:259:GLN:OE1 | 2:D:327:PRO:HA | 0.55 | 2.02 | 2 | 1 |
| 1:A:18:VAL:HG11 | 1:A:51:ILE:HD12 | 0.55 | 1.78 | 9 | 2 |
| 1:A:29:LEU:HG | 1:C:225:HIS:CB | 0.55 | 2.32 | 1 | 4 |
| 1:C:258:ILE:O | 1:C:262:LEU:HG | 0.55 | 2.02 | 12 | 4 |
| 1:C:254:LYS:HA | 1:C:259:GLN:NE2 | 0.55 | 2.17 | 17 | 6 |
| 1:C:237:GLN:HE21 | 1:C:237:GLN:N | 0.55 | 2.00 | 7 | 1 |
| 1:C:222:ASN:ND2 | 1:C:242:LEU:HD12 | 0.54 | 2.17 | 8 | 1 |
| 1:C:229:LEU:O | 1:C:237:GLN:HB2 | 0.54 | 2.02 | 13 | 1 |
| 1:C:216:SER:HB2 | 2:D:324:MET:H | 0.54 | 1.62 | 15 | 1 |
| 1:C:236:CYS:O | 1:C:253:PRO:HG3 | 0.54 | 2.03 | 20 | 5 |
| 1:C:211:CYS:HB3 | 1:C:237:GLN:OE1 | 0.54 | 2.02 | 3 | 1 |
| 1:A:36:CYS:O | 1:A:53:PRO:HG3 | 0.54 | 2.03 | 4 | 6 |
| 2:B:123:SER:O | 2:B:124:MET:HG3 | 0.54 | 2.02 | 18 | 1 |
| 1:A:28:ILE:O | 1:C:225:HIS:HB2 | 0.53 | 2.03 | 15 | 3 |
| 1:A:14:PHE:CD1 | 1:A:52:ASP:HB2 | 0.53 | 2.39 | 16 | 3 |
| 1:A:15:GLU:OE2 | 1:A:49:VAL:HG11 | 0.53 | 2.04 | 19 | 1 |
| 2:D:325:LYS:HD3 | 2:D:326:GLU:N | 0.53 | 2.18 | 13 | 1 |
| 1:C:231:THR:OG1 | 1:C:234:CYS:HB2 | 0.53 | 2.02 | 8 | 3 |
| 1:C:255:LEU:O | 1:C:259:GLN:HG2 | 0.53 | 2.04 | 1 | 10 |
| 2:B:120:ASP:O | 2:B:123:SER:HB2 | 0.52 | 2.04 | 5 | 3 |
| 1:A:24:LYS:CG | 1:A:43:LYS:HB3 | 0.52 | 2.34 | 11 | 1 |
| 1:A:17:HIS:O | 1:A:18:VAL:HB | 0.52 | 2.04 | 11 | 1 |
| 1:C:215:GLU:HA | 2:D:320:ASP:O | 0.52 | 2.05 | 8 | 1 |
| 2:D:320:ASP:O | 2:D:323:SER:HB2 | 0.52 | 2.05 | 9 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:C:220:ARG:O | 1:C:220:ARG:HD2 | 0.52 | 2.04 | 14 | 1 |
| 1:A:31:THR:OG1 | 1:A:34:CYS:HB2 | 0.51 | 2.06 | 1 | 3 |
| 1:A:16:SER:O | 1:A:55:LEU:HD11 | 0.51 | 2.06 | 15 | 3 |
| 1:A:47:ARG:CZ | 1:A:49:VAL:HG12 | 0.51 | 2.35 | 3 | 7 |
| 1:C:214:PHE:O | 2:D:323:SER:HA | 0.51 | 2.06 | 19 | 1 |
| 1:C:214:PHE:CD1 | 1:C:252:ASP:HB2 | 0.51 | 2.40 | 1 | 1 |
| 1:C:247:ARG:NH1 | 1:C:249:VAL:HG12 | 0.51 | 2.21 | 14 | 1 |
| 1:C:247:ARG:NH1 | 1:C:249:VAL:HG11 | 0.50 | 2.21 | 16 | 1 |
| 1:A:55:LEU:O | 1:A:59:GLN:HG2 | 0.50 | 2.06 | 13 | 11 |
| 1:A:15:GLU:OE1 | 1:A:49:VAL:HB | 0.50 | 2.06 | 9 | 2 |
| 1:C:225:HIS:O | 1:C:240:ALA:HA | 0.50 | 2.07 | 5 | 1 |
| 1:A:25:HIS:HD2 | 1:C:229:LEU:HD13 | 0.50 | 1.66 | 10 | 1 |
| 1:C:231:THR:OG1 | 1:C:234:CYS:HB3 | 0.50 | 2.07 | 19 | 1 |
| 1:A:56:LYS:O | 1:A:60:GLU:HG2 | 0.50 | 2.06 | 9 | 5 |
| 1:C:256:LYS:O | 1:C:260:GLU:HG2 | 0.50 | 2.07 | 9 | 3 |
| 1:C:254:LYS:O | 2:D:327:PRO:HA | 0.50 | 2.07 | 16 | 2 |
| 1:A:25:HIS:HB2 | 1:C:228:ILE:O | 0.50 | 2.06 | 10 | 3 |
| 1:A:25:HIS:CD2 | 1:C:229:LEU:HD13 | 0.50 | 2.42 | 10 | 1 |
| 1:C:220:ARG:HB3 | 1:C:257:TRP:CD2 | 0.50 | 2.41 | 16 | 2 |
| 1:C:259:GLN:HE21 | 1:C:259:GLN:HA | 0.49 | 1.67 | 2 | 1 |
| 1:C:252:ASP:OD1 | 1:C:254:LYS:HB2 | 0.49 | 2.08 | 6 | 4 |
| 1:A:48:GLN:H | 1:A:48:GLN:HE21 | 0.49 | 1.49 | 1 | 1 |
| 1:C:216:SER:O | 1:C:255:LEU:HD11 | 0.49 | 2.07 | 3 | 1 |
| 1:C:252:ASP:O | 1:C:255:LEU:HB2 | 0.49 | 2.07 | 16 | 4 |
| 1:A:52:ASP:OD2 | 1:A:54:LYS:HB2 | 0.49 | 2.07 | 12 | 2 |
| 1:C:229:LEU:O | 1:C:237:GLN:HB3 | 0.49 | 2.08 | 20 | 2 |
| 1:C:264:LYS:HE2 | 1:C:264:LYS:HA | 0.49 | 1.84 | 15 | 1 |
| 2:D:323:SER:O | 2:D:324:MET:HG3 | 0.48 | 2.08 | 6 | 1 |
| 1:C:251:ILE:CG2 | 1:C:255:LEU:HD12 | 0.48 | 2.38 | 12 | 1 |
| 1:A:59:GLN:HA | 1:C:266:LEU:CD2 | 0.48 | 2.38 | 1 | 2 |
| 1:C:254:LYS:HB3 | 2:D:327:PRO:HD3 | 0.48 | 1.84 | 1 | 2 |
| 1:A:22:ASN:O | 1:A:43:LYS:HG2 | 0.48 | 2.09 | 10 | 3 |
| 1:A:47:ARG:NH1 | 1:A:49:VAL:HG12 | 0.48 | 2.23 | 12 | 1 |
| 1:A:52:ASP:OD1 | 1:A:54:LYS:HB2 | 0.48 | 2.09 | 19 | 3 |
| 1:A:12:ARG:NE | 1:A:12:ARG:HA | 0.48 | 2.24 | 5 | 2 |
| 1:C:227:LYS:NZ | 1:C:227:LYS:HB3 | 0.48 | 2.24 | 19 | 1 |
| 1:A:61:TYR:O | 1:A:64:LYS:HG2 | 0.47 | 2.08 | 16 | 1 |
| 2:D:326:GLU:HB2 | 2:D:327:PRO:CD | 0.47 | 2.40 | 1 | 1 |
| 1:C:242:LEU:HD23 | 1:C:247:ARG:O | 0.47 | 2.10 | 14 | 2 |
| 1:A:14:PHE:CD2 | 1:A:52:ASP:HB2 | 0.47 | 2.45 | 20 | 1 |
| 1:C:254:LYS:HB2 | 1:C:254:LYS:HZ2 | 0.47 | 1.68 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 2:D:326:GLU:HB3 | 2:D:327:PRO:HD2 | 0.47 | 1.87 | 7 | 1 |
| 1:C:232:PRO:O | 1:C:233:ASN:HB2 | 0.47 | 2.09 | 9 | 1 |
| 1:A:48:GLN:H | 1:A:48:GLN:NE2 | 0.46 | 2.07 | 1 | 1 |
| 1:A:66:LEU:HD21 | 1:C:259:GLN:HA | 0.46 | 1.86 | 16 | 2 |
| 1:A:11:CYS:HB2 | 1:A:37:GLN:OE1 | 0.46 | 2.10 | 6 | 2 |
| 1:A:24:LYS:CG | 1:A:43:LYS:HA | 0.46 | 2.41 | 7 | 3 |
| 1:C:215:GLU:OE1 | 1:C:249:VAL:HB | 0.46 | 2.11 | 14 | 1 |
| 2:B:126:GLU:HB2 | 2:B:127:PRO:HD2 | 0.46 | 1.87 | 6 | 1 |
| 1:C:222:ASN:O | 1:C:243:LYS:HG3 | 0.46 | 2.11 | 7 | 3 |
| 1:C:224:LYS:HG3 | 1:C:243:LYS:HA | 0.46 | 1.86 | 19 | 1 |
| 1:A:52:ASP:O | 1:A:55:LEU:HB2 | 0.46 | 2.11 | 17 | 5 |
| 1:A:16:SER:HB2 | 2:B:125:LYS:CG | 0.46 | 2.40 | 19 | 1 |
| 1:A:15:GLU:HA | 2:B:120:ASP:O | 0.45 | 2.10 | 13 | 1 |
| 1:A:16:SER:HA | 1:A:55:LEU:HD11 | 0.45 | 1.89 | 15 | 1 |
| 1:C:215:GLU:OE2 | 2:D:319:GLY:HA2 | 0.45 | 2.11 | 8 | 1 |
| 2:B:125:LYS:HD2 | 2:B:126:GLU:N | 0.45 | 2.26 | 6 | 1 |
| 1:A:16:SER:OG | 2:B:125:LYS:HB2 | 0.45 | 2.12 | 16 | 1 |
| 1:C:240:ALA:HB2 | 1:C:251:ILE:HD12 | 0.45 | 1.88 | 5 | 1 |
| 1:A:22:ASN:O | 1:A:43:LYS:HG3 | 0.45 | 2.11 | 16 | 2 |
| 1:C:229:LEU:HB2 | 1:C:237:GLN:HB2 | 0.45 | 1.89 | 10 | 1 |
| 1:A:51:ILE:HD12 | 1:A:58:ILE:HD11 | 0.45 | 1.87 | 17 | 1 |
| 1:C:209:CYS:SG | 1:C:233:ASN:HB3 | 0.45 | 2.52 | 1 | 1 |
| 1:C:254:LYS:HB2 | 1:C:254:LYS:NZ | 0.45 | 2.26 | 12 | 2 |
| 1:A:48:GLN:HE21 | 1:A:48:GLN:N | 0.45 | 2.10 | 1 | 1 |
| 1:A:38:ILE:HG22 | 1:A:51:ILE:HD11 | 0.45 | 1.89 | 20 | 2 |
| 1:A:54:LYS:HD2 | 2:B:127:PRO:HD3 | 0.45 | 1.87 | 6 | 2 |
| 1:A:27:LYS:HB2 | 1:A:27:LYS:NZ | 0.45 | 2.26 | 10 | 1 |
| 1:A:61:TYR:OH | 1:C:230:ASN:HB2 | 0.45 | 2.12 | 4 | 2 |
| 1:A:66:LEU:CD2 | 1:C:259:GLN:HA | 0.44 | 2.41 | 3 | 3 |
| 1:C:248:GLN:HE21 | 1:C:248:GLN:N | 0.44 | 2.10 | 1 | 1 |
| 1:C:215:GLU:HG3 | 2:D:320:ASP:O | 0.44 | 2.12 | 16 | 1 |
| 1:A:54:LYS:HB3 | 2:B:127:PRO:HD3 | 0.44 | 1.88 | 1 | 2 |
| 1:A:24:LYS:HG2 | 1:A:43:LYS:HB3 | 0.44 | 1.89 | 3 | 1 |
| 1:C:254:LYS:NZ | 1:C:254:LYS:HB2 | 0.44 | 2.28 | 13 | 1 |
| 1:C:254:LYS:O | 2:D:327:PRO:HB3 | 0.44 | 2.13 | 1 | 1 |
| 1:A:58:ILE:O | 1:A:62:LEU:HG | 0.44 | 2.12 | 12 | 6 |
| 1:A:24:LYS:HG3 | 1:A:43:LYS:HA | 0.44 | 1.89 | 19 | 1 |
| 1:C:238:ILE:HG22 | 1:C:251:ILE:HD11 | 0.44 | 1.90 | 20 | 1 |
| 1:A:20:ARG:HD2 | 1:A:20:ARG:O | 0.43 | 2.13 | 14 | 1 |
| 2:B:119:GLY:HA2 | 2:B:123:SER:CB | 0.43 | 2.43 | 18 | 1 |
| 1:C:254:LYS:HE2 | 2:D:325:LYS:O | 0.43 | 2.13 | 20 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:64:LYS:HD3 | 1:A:65:CYS:N | 0.43 | 2.28 | 17 | 2 |
| 1:C:222:ASN:HD22 | 1:C:242:LEU:HD12 | 0.43 | 1.72 | 8 | 1 |
| 1:A:67:ASN:HA | 1:C:254:LYS:HE3 | 0.43 | 1.89 | 14 | 1 |
| 1:C:257:TRP:O | 1:C:261:TYR:HB2 | 0.43 | 2.14 | 13 | 1 |
| 1:A:54:LYS:HB3 | 2:B:127:PRO:N | 0.43 | 2.28 | 19 | 1 |
| 1:A:29:LEU:HG | 1:C:225:HIS:HB3 | 0.43 | 1.90 | 1 | 1 |
| 1:C:247:ARG:NH1 | 1:C:249:VAL:HA | 0.43 | 2.28 | 12 | 2 |
| 1:C:212:ARG:HA | 1:C:212:ARG:HE | 0.43 | 1.73 | 5 | 1 |
| 1:C:221:ALA:O | 1:C:243:LYS:HD3 | 0.43 | 2.14 | 11 | 1 |
| 1:C:264:LYS:NZ | 1:C:264:LYS:HB2 | 0.43 | 2.28 | 13 | 1 |
| 1:C:222:ASN:C | 1:C:243:LYS:HG2 | 0.43 | 2.34 | 17 | 1 |
| 1:A:12:ARG:O | 1:A:12:ARG:HD3 | 0.43 | 2.14 | 6 | 1 |
| 1:A:9:CYS:SG | 1:A:33:ASN:HB3 | 0.43 | 2.54 | 7 | 1 |
| 1:A:59:GLN:NE2 | 1:C:266:LEU:HD13 | 0.43 | 2.28 | 10 | 1 |
| 1:C:214:PHE:HB3 | 1:C:250:CYS:SG | 0.43 | 2.53 | 14 | 1 |
| 1:C:254:LYS:HA | 1:C:259:GLN:OE1 | 0.43 | 2.13 | 10 | 1 |
| 1:A:16:SER:O | 1:A:55:LEU:HD21 | 0.43 | 2.13 | 17 | 1 |
| 1:A:28:ILE:HA | 1:A:37:GLN:O | 0.43 | 2.14 | 2 | 1 |
| 1:C:222:ASN:O | 1:C:243:LYS:HG2 | 0.43 | 2.13 | 3 | 1 |
| 1:C:214:PHE:CD1 | 1:C:252:ASP:HA | 0.43 | 2.48 | 9 | 1 |
| 1:C:216:SER:HA | 1:C:255:LEU:HD11 | 0.43 | 1.90 | 15 | 1 |
| 1:C:210:PRO:HD2 | 1:C:237:GLN:OE1 | 0.42 | 2.13 | 18 | 1 |
| 1:C:254:LYS:CB | 2:D:327:PRO:HD3 | 0.42 | 2.44 | 1 | 1 |
| 1:C:266:LEU:O | 1:C:267:ASN:HB2 | 0.42 | 2.14 | 10 | 1 |
| 1:A:12:ARG:HD3 | 1:A:13:PHE:CE2 | 0.42 | 2.49 | 14 | 1 |
| 1:A:66:LEU:HD23 | 1:C:262:LEU:HB2 | 0.42 | 1.91 | 16 | 1 |
| 1:A:47:ARG:NH2 | 1:A:49:VAL:HA | 0.42 | 2.29 | 3 | 1 |
| 1:C:254:LYS:HA | 1:C:259:GLN:HE22 | 0.42 | 1.75 | 4 | 1 |
| 1:C:237:GLN:HA | 1:C:237:GLN:HE21 | 0.42 | 1.74 | 14 | 1 |
| 1:C:255:LEU:HD23 | 2:D:325:LYS:HG3 | 0.42 | 1.90 | 20 | 1 |
| 1:A:25:HIS:CB | 1:C:229:LEU:HG | 0.42 | 2.45 | 6 | 1 |
| 1:C:259:GLN:O | 1:C:263:GLU:HB2 | 0.42 | 2.14 | 10 | 1 |
| 1:C:238:ILE:HB | 1:C:251:ILE:HG13 | 0.42 | 1.92 | 17 | 1 |
| 1:A:51:ILE:H | 1:A:51:ILE:HD13 | 0.41 | 1.76 | 11 | 1 |
| 1:C:247:ARG:CZ | 1:C:249:VAL:HG12 | 0.41 | 2.46 | 7 | 2 |
| 1:A:16:SER:HA | 1:A:55:LEU:HD21 | 0.41 | 1.92 | 7 | 1 |
| 1:A:20:ARG:HA | 1:A:23:VAL:HG22 | 0.41 | 1.92 | 9 | 1 |
| 1:C:211:CYS:HB2 | 1:C:237:GLN:OE1 | 0.41 | 2.15 | 15 | 1 |
| 1:A:38:ILE:HB | 1:A:51:ILE:HG12 | 0.41 | 1.92 | 13 | 3 |
| 1:A:15:GLU:HG3 | 1:A:49:VAL:HB | 0.41 | 1.92 | 16 | 1 |
| 1:C:242:LEU:HD21 | 1:C:249:VAL:HG13 | 0.41 | 1.92 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:17:HIS:CE1 | 2:B:125:LYS:HE3 | 0.41 | 2.50 | 5 | 1 |
| 2:B:125:LYS:HD2 | 2:B:126:GLU:O | 0.41 | 2.15 | 6 | 1 |
| 1:A:64:LYS:NZ | 1:A:64:LYS:HB3 | 0.41 | 2.31 | 9 | 1 |
| 1:A:16:SER:HB3 | 2:B:125:LYS:HB2 | 0.41 | 1.92 | 11 | 1 |
| 1:C:239:VAL:HG22 | 1:C:250:CYS:SG | 0.41 | 2.56 | 19 | 1 |
| 1:C:251:ILE:HD13 | 1:C:251:ILE:H | 0.41 | 1.76 | 1 | 1 |
| 1:C:216:SER:O | 1:C:255:LEU:HG | 0.41 | 2.16 | 5 | 1 |
| 1:A:67:ASN:ND2 | 2:D:327:PRO:HG3 | 0.41 | 2.31 | 7 | 1 |
| 2:B:126:GLU:HB3 | 2:B:127:PRO:HD2 | 0.41 | 1.92 | 7 | 2 |
| 1:A:26:LEU:O | 1:C:227:LYS:HG3 | 0.41 | 2.15 | 10 | 1 |
| 1:C:216:SER:HB2 | 2:D:325:LYS:HB2 | 0.41 | 1.92 | 18 | 1 |
| 1:C:220:ARG:HG2 | 1:C:257:TRP:CE3 | 0.40 | 2.51 | 14 | 1 |
| 1:C:217:HIS:HB2 | 2:D:322:ASP:OD2 | 0.40 | 2.16 | 15 | 1 |
| 1:C:237:GLN:HE21 | 1:C:237:GLN:HA | 0.40 | 1.76 | 18 | 1 |
| 1:C:251:ILE:N | 1:C:251:ILE:HD13 | 0.40 | 2.31 | 11 | 1 |
| 1:C:224:LYS:HG2 | 1:C:243:LYS:HB3 | 0.40 | 1.93 | 11 | 1 |
| 1:A:17:HIS:HB2 | 2:B:122:ASP:OD1 | 0.40 | 2.16 | 16 | 1 |
| 1:C:215:GLU:CG | 1:C:218:VAL:HB | 0.40 | 2.46 | 18 | 1 |
| 1:A:15:GLU:OE1 | 1:A:18:VAL:HB | 0.40 | 2.16 | 19 | 1 |
| 1:C:252:ASP:HB3 | 1:C:255:LEU:HG | 0.40 | 1.93 | 2 | 1 |
| 1:A:14:PHE:CE1 | 1:A:52:ASP:HB2 | 0.40 | 2.51 | 13 | 1 |
| 1:C:261:TYR:O | 1:C:264:LYS:HG3 | 0.40 | 2.16 | 3 | 1 |
| 1:A:20:ARG:HB3 | 1:A:57:TRP:CZ3 | 0.40 | 2.50 | 17 | 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 | 57/70 (81%) | 51±3 (90±5%) | 5±2 (9±4%) | 1±1 (2±2%) | 12 | 54 |
| 1 | C | 56/70 (80%) | 51±2 (91±3%) | 4±1 (7±2%) | 1±1 (2±2%) | 10 | 49 |
| 2 | B | 8/40 (20%) | 5±1 (59±14%) | 3±1 (38±13%) | 0±1 (4±7%) | 5 | 33 |
| 2 | D | 8/40 (20%) | 5±1 (57±16%) | 3±1 (35±14%) | 1±1 (8±9%) | 2 | 15 |
| All | All | 2580/4400 (59%) | 2222 (86%) | 294 (11%) | 64 (2%) | 9 | 45 |

All 25 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | C | 210 | PRO | 10 |
| 1 | A | 10 | PRO | 6 |
| 1 | A | 35 | ALA | 4 |
| 1 | C | 233 | ASN | 3 |
| 1 | C | 243 | LYS | 3 |
| 1 | C | 256 | LYS | 3 |
| 1 | A | 43 | LYS | 3 |
| 2 | D | 324 | MET | 3 |
| 1 | A | 67 | ASN | 3 |
| 2 | D | 323 | SER | 3 |
| 2 | D | 327 | PRO | 2 |
| 1 | C | 235 | ALA | 2 |
| 1 | C | 232 | PRO | 2 |
| 1 | A | 55 | LEU | 2 |
| 2 | B | 123 | SER | 2 |
| 2 | B | 126 | GLU | 2 |
| 2 | D | 326 | GLU | 2 |
| 2 | B | 119 | GLY | 2 |
| 1 | A | 47 | ARG | 1 |
| 1 | A | 32 | PRO | 1 |
| 2 | D | 322 | ASP | 1 |
| 1 | C | 267 | ASN | 1 |
| 1 | A | 18 | VAL | 1 |
| 1 | C | 218 | VAL | 1 |
| 2 | D | 320 | ASP | 1 |

### 6.3.2 Protein sidechains (i)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 53/65 (82%) | 50±2 (94±3%) | 3±2 (6±3%) | 21 | 70 |
| 1 | C | 52/65 (80%) | 48±3 (93±5%) | 4±3 (7±5%) | 18 | 67 |
| 2 | B | 7/31 (23%) | 7±1 (96±8%) | 0±1 (4±8%) | 33 | 81 |
| 2 | D | 7/31 (23%) | 7±1 (96±8%) | 0±1 (4±8%) | 33 | 81 |
| All | All | 2380/3840 (62%) | 2227 (94%) | 153 (6%) | 21 | 70 |

All 46 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 | 47 | ARG | 9 |
| 1 | A | 64 | LYS | 9 |
| 1 | C | 215 | GLU | 8 |
| 1 | A | 15 | GLU | 7 |
| 1 | C | 264 | LYS | 7 |
| 1 | C | 230 | ASN | 6 |
| 1 | C | 251 | ILE | 6 |
| 1 | C | 247 | ARG | 6 |
| 1 | A | 51 | ILE | 6 |
| 1 | A | 12 | ARG | 5 |
| 1 | A | 55 | LEU | 5 |
| 1 | C | 212 | ARG | 5 |
| 1 | C | 237 | GLN | 5 |
| 1 | A | 37 | GLN | 5 |
| 1 | A | 48 | GLN | 4 |
| 1 | A | 66 | LEU | 4 |
| 1 | C | 248 | GLN | 4 |
| 1 | A | 20 | ARG | 4 |
| 1 | C | 266 | LEU | 4 |
| 1 | C | 267 | ASN | 4 |
| 1 | C | 263 | GLU | 3 |
| 2 | B | 126 | GLU | 3 |
| 2 | D | 324 | MET | 2 |
| 1 | C | 255 | LEU | 2 |
| 2 | B | 125 | LYS | 2 |
| 1 | A | 14 | PHE | 2 |
| 1 | C | 214 | PHE | 2 |
| 1 | C | 233 | ASN | 2 |
| 1 | C | 220 | ARG | 2 |
| 2 | D | 326 | GLU | 2 |
| 2 | D | 325 | LYS | 2 |
| 1 | A | 30 | ASN | 2 |
| 1 | C | 256 | LYS | 1 |
| 1 | C | 259 | GLN | 1 |
| 1 | C | 225 | HIS | 1 |
| 1 | A | 25 | HIS | 1 |
| 1 | A | 27 | LYS | 1 |
| 1 | C | 229 | LEU | 1 |
| 1 | C | 243 | LYS | 1 |
| 1 | A | 56 | LYS | 1 |
| 1 | C | 227 | LYS | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 42 | LEU | 1 |
| 1 | C | 222 | ASN | 1 |
| 1 | C | 242 | LEU | 1 |
| 2 | B | 124 | MET | 1 |
| 1 | A | 63 | GLU | 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)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | TYS | D | 321 | 2 | 15,16,17 | 2.59±0.16 | 1±0 (9±3%) |
| 2 | TYS | D | 312 | 2 | 15,16,17 | 2.62±0.19 | 2±0 (10±3%) |
| 2 | TYS | B | 107 | 2 | 15,16,17 | 2.66±0.20 | 2±0 (10±3%) |
| 2 | TYS | D | 307 | 2 | 15,16,17 | 2.69±0.28 | 2±0 (10±3%) |
| 2 | TYS | B | 112 | 2 | 15,16,17 | 2.56±0.17 | 2±1 (10±3%) |
| 2 | TYS | B | 121 | 2 | 15,16,17 | 2.58±0.17 | 1±0 (8±3%) |

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

| Mol | Type | Chain | Res | Link | Bond angles | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | TYS | D | 321 | 2 | 18,22,24 | 1.03±0.05 | 2±0 (8±2%) |
| 2 | TYS | D | 312 | 2 | 18,22,24 | 1.06±0.07 | 2±1 (11±4%) |
| 2 | TYS | B | 107 | 2 | 18,22,24 | 1.03±0.08 | 2±0 (8±2%) |
| 2 | TYS | D | 307 | 2 | 18,22,24 | 1.04±0.07 | 1±0 (8±2%) |
| 2 | TYS | B | 112 | 2 | 18,22,24 | 1.04±0.04 | 2±1 (8±3%) |
| 2 | TYS | B | 121 | 2 | 18,22,24 | 1.02±0.06 | 2±0 (8±2%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | TYS | D | 321 | 2 | - | 0±0,10,11,13 | 0±0,1,1,1 |
| 2 | TYS | B | 112 | 2 | - | 0±0,10,11,13 | 0±0,1,1,1 |
| 2 | TYS | B | 121 | 2 | - | 0±0,10,11,13 | 0±0,1,1,1 |
| 2 | TYS | D | 312 | 2 | - | 0±0,10,11,13 | 0±0,1,1,1 |
| 2 | TYS | D | 307 | 2 | - | 0±0,10,11,13 | 0±0,1,1,1 |
| 2 | TYS | B | 107 | 2 | - | 0±0,10,11,13 | 0±0,1,1,1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 2 | D | 307 | TYS | OH-S | 11.84 | 1.40 | 1.58 | 14 | 20 |
| 2 | B | 107 | TYS | OH-S | 11.00 | 1.41 | 1.58 | 14 | 20 |
| 2 | B | 121 | TYS | OH-S | 10.79 | 1.41 | 1.58 | 6 | 20 |
| 2 | D | 312 | TYS | OH-S | 10.63 | 1.42 | 1.58 | 2 | 20 |
| 2 | B | 112 | TYS | OH-S | 10.57 | 1.42 | 1.58 | 1 | 20 |
| 2 | D | 321 | TYS | OH-S | 10.49 | 1.42 | 1.58 | 8 | 20 |
| 2 | D | 307 | TYS | OH-CZ | 4.18 | 1.35 | 1.42 | 14 | 10 |
| 2 | B | 107 | TYS | OH-CZ | 3.13 | 1.37 | 1.42 | 14 | 11 |
| 2 | B | 112 | TYS | OH-CZ | 2.85 | 1.37 | 1.42 | 19 | 9 |
| 2 | D | 312 | TYS | OH-CZ | 2.80 | 1.38 | 1.42 | 10 | 11 |
| 2 | B | 107 | TYS | CB-CA | 2.70 | 1.59 | 1.53 | 13 | 1 |
| 2 | D | 321 | TYS | OH-CZ | 2.55 | 1.38 | 1.42 | 8 | 7 |
| 2 | B | 112 | TYS | CA-N | 2.48 | 1.40 | 1.48 | 15 | 1 |
| 2 | B | 121 | TYS | OH-CZ | 2.44 | 1.38 | 1.42 | 13 | 6 |
| 2 | D | 307 | TYS | CE2-CD2 | 2.20 | 1.34 | 1.38 | 16 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 2 | D | 312 | TYS | OH-S-O2 | 3.20 | 117.03 | 107.71 | 3 | 20 |
| 2 | B | 121 | TYS | OH-S-O2 | 3.15 | 116.90 | 107.71 | 19 | 20 |
| 2 | B | 107 | TYS | OH-S-O2 | 3.09 | 116.72 | 107.71 | 7 | 20 |
| 2 | B | 112 | TYS | OH-S-O2 | 3.05 | 116.59 | 107.71 | 15 | 20 |
| 2 | D | 321 | TYS | OH-S-O2 | 2.98 | 116.40 | 107.71 | 5 | 20 |
| 2 | D | 307 | TYS | OH-S-O2 | 2.90 | 116.17 | 107.71 | 17 | 20 |
| 2 | B | 107 | TYS | CB-CA-C | 2.76 | 106.30 | 111.47 | 20 | 2 |
| 2 | D | 307 | TYS | CB-CA-C | 2.66 | 106.47 | 111.47 | 20 | 2 |
| 2 | D | 312 | TYS | CB-CA-C | 2.64 | 106.52 | 111.47 | 16 | 1 |
| 2 | D | 312 | TYS | O3-S-O2 | 2.56 | 99.60 | 108.49 | 9 | 14 |
| 2 | D | 312 | TYS | OH-S-O1 | 2.36 | 114.59 | 107.71 | 16 | 6 |
| 2 | B | 112 | TYS | O3-S-O2 | 2.35 | 100.32 | 108.49 | 7 | 9 |
| 2 | D | 307 | TYS | O3-S-O2 | 2.32 | 100.44 | 108.49 | 13 | 7 |
| 2 | B | 107 | TYS | O3-S-O2 | 2.30 | 100.51 | 108.49 | 7 | 9 |
| 2 | B | 121 | TYS | CB-CA-C | 2.24 | 107.28 | 111.47 | 6 | 1 |
| 2 | B | 121 | TYS | O3-S-O2 | 2.21 | 100.82 | 108.49 | 20 | 9 |
| 2 | D | 321 | TYS | O3-S-O2 | 2.18 | 100.93 | 108.49 | 2 | 10 |
| 2 | B | 112 | TYS | OH-S-O1 | 2.15 | 113.99 | 107.71 | 4 | 1 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 88% for the well-defined parts and 85% 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 | 2494 |
| Number of shifts mapped to atoms | 2494 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 2 |

### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 198 | -0.46 ± 0.06 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 190 | -0.43 ± 0.07 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 182 | -0.25 ± 0.09 | None needed (< 0.5 ppm) |
| $^{15}N$ | 188 | -0.50 ± 0.28 | None needed (imprecise) |

### 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 88%, i.e. 1628 atoms were assigned a chemical shift out of a possible 1845. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 609/631 (97%) | 248/252 (98%) | 240/258 (93%) | 121/121 (100%) |
| Sidechain | 943/1100 (86%) | 644/709 (91%) | 285/336 (85%) | 14/55 (25%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 76/114 (67%) | 44/56 (79%) | 30/48 (62%) | 2/10 (20%) |
| Overall | 1628/1845 (88%) | 936/1017 (92%) | 555/642 (86%) | 137/186 (74%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 2410 atoms were assigned a chemical shift out of a possible 2840. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 958/1016 (94%) | 390/408 (96%) | 380/412 (92%) | 188/196 (96%) |
| Sidechain | 1336/1652 (81%) | 912/1058 (86%) | 408/510 (80%) | 16/84 (19%) |
| Aromatic | 116/172 (67%) | 70/84 (83%) | 44/78 (56%) | 2/10 (20%) |
| Overall | 2410/2840 (85%) | 1372/1550 (89%) | 832/1000 (83%) | 206/290 (71%) |

### 7.1.4 Statistically unusual chemical shifts (i)

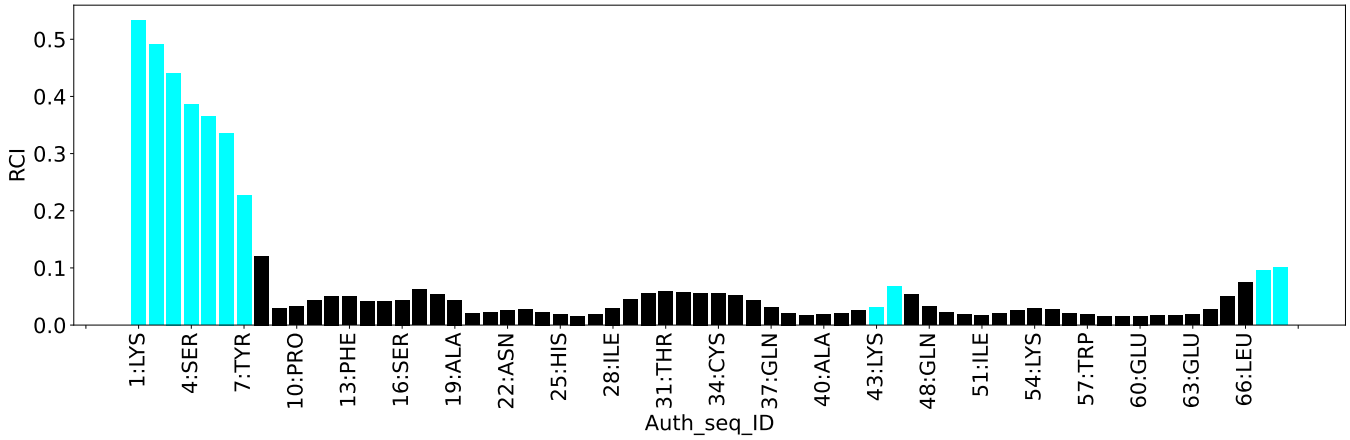
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, *ppm* | Expected range, *ppm* | Z-score |
|---|---|---|---|---|---|---|---|
| 1 | A | 20 | ARG | HB3 | 0.41 | 0.43 – 3.11 | -5.1 |
| 1 | C | 220 | ARG | HB3 | 0.41 | 0.43 – 3.11 | -5.1 |

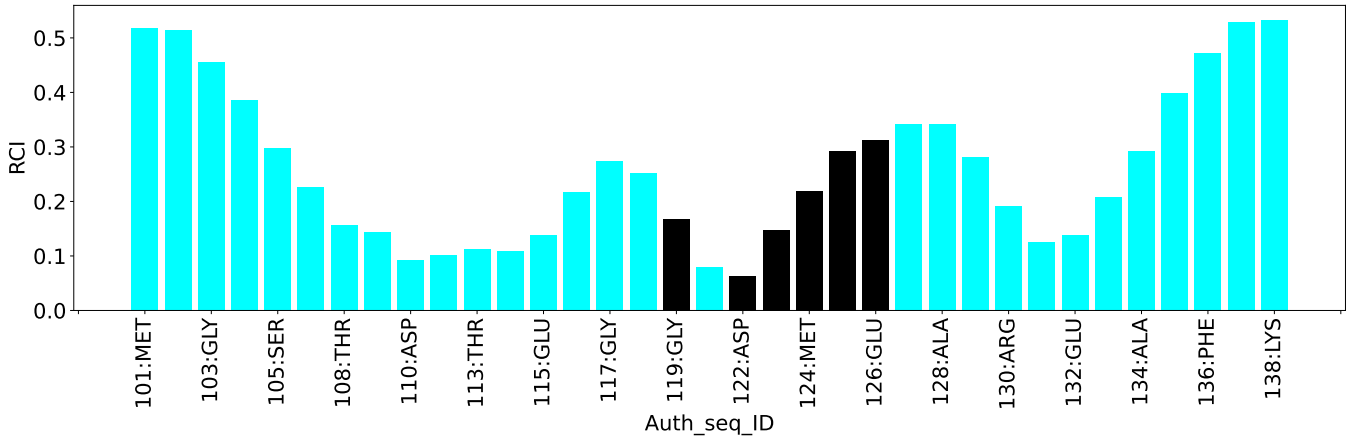
### 7.1.5 Random Coil Index (RCI) plots (i)

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.

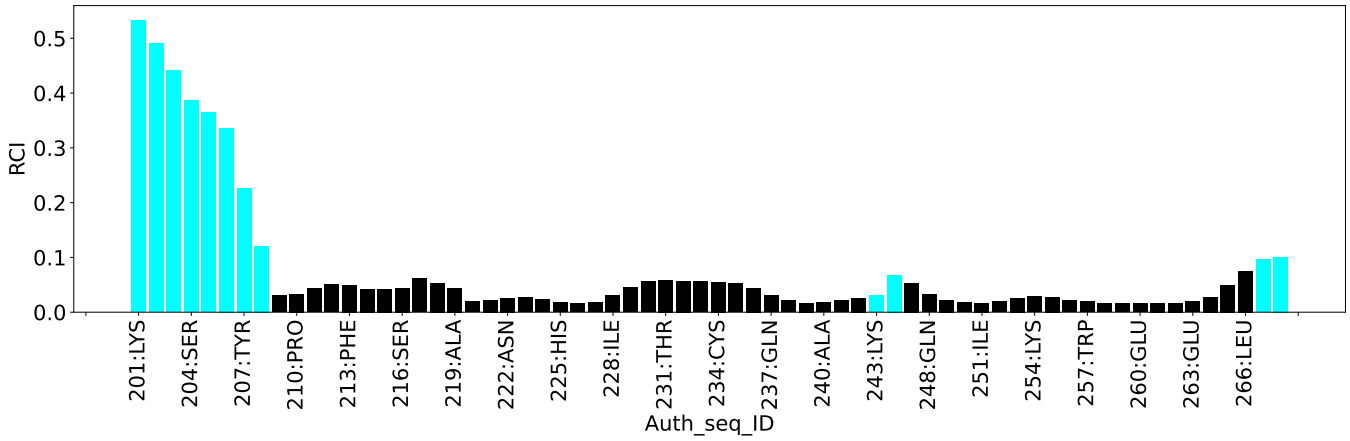
Random coil index (RCI) for chain A:



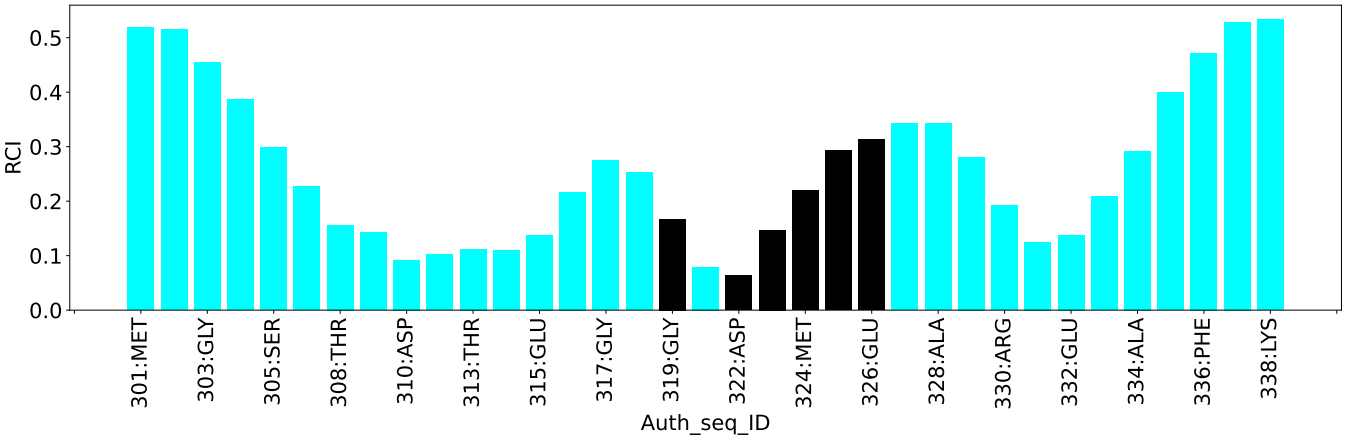

Random coil index (RCI) for chain B:




Random coil index (RCI) for chain C:




Random coil index (RCI) for chain D:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
301:MET
303:GLY
305:SER
308:THR
310:ASP
313:THR
315:GLU
317:GLY
319:GLY
322:ASP
324:MET
326:GLU
328:ALA
330:ARG
332:GLU
334:ALA
336:PHE
338:LYS
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 | 1687 |
| Intra-residue (\|i-j\|=0) | 560 |
| Sequential (\|i-j\|=1) | 379 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 197 |
| Long range (\|i-j\|≥5) | 368 |
| Inter-chain | 183 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 128 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 8.2 |
| Number of long range restraints per residue[1] | 1.7 |

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

## 8.2 Residual restraint violations (i)

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

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

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

| Bins (Å) | Average number of violations per model | Max (Å) |
|---|---|---|
| 0.1-0.2 (Small) | 35.8 | 0.2 |
| 0.2-0.5 (Medium) | 34.8 | 0.5 |
| >0.5 (Large) | 34.0 | 4.35 |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|---|---|---|
| 1.0-10.0 (Small) | 15.9 | 4.94 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

# 9 Distance violation analysis (i)

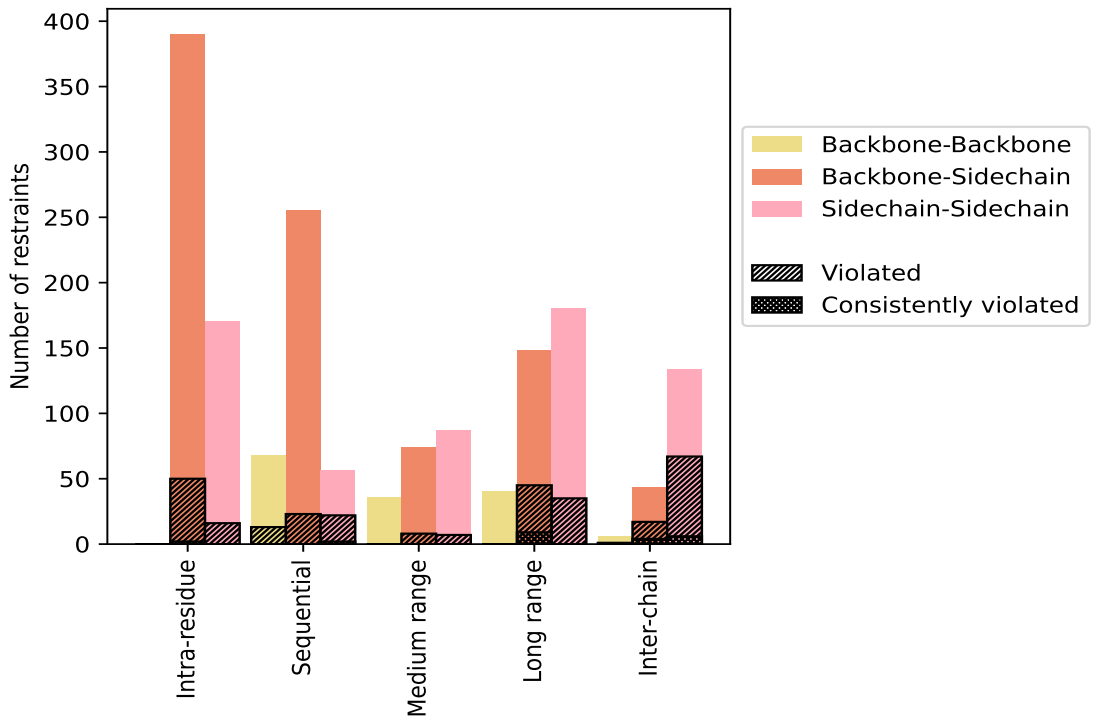
## 9.1 Summary of distance violations (i)

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

| Restraints type | Count | %[1] | Violated[3] | | | Consistently Violated[4] | | |
|---|---|---|---|---|---|---|---|---|
| | | | Count | %[2] | %[1] | Count | %[2] | %[1] |
| Intra-residue (\|i-j\|=0) | 560 | 33.2 | 66 | 11.8 | 3.9 | 2 | 0.4 | 0.1 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 390 | 23.1 | 50 | 12.8 | 3.0 | 2 | 0.5 | 0.1 |
| Sidechain-Sidechain | 170 | 10.1 | 16 | 9.4 | 0.9 | 0 | 0.0 | 0.0 |
| Sequential (\|i-j\|=1) | 379 | 22.5 | 58 | 15.3 | 3.4 | 2 | 0.5 | 0.1 |
| Backbone-Backbone | 68 | 4.0 | 13 | 19.1 | 0.8 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 255 | 15.1 | 23 | 9.0 | 1.4 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 56 | 3.3 | 22 | 39.3 | 1.3 | 2 | 3.6 | 0.1 |
| Medium range (\|i-j\|>1 & \|i-j\|<5) | 197 | 11.7 | 15 | 7.6 | 0.9 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 36 | 2.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 74 | 4.4 | 8 | 10.8 | 0.5 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 87 | 5.2 | 7 | 8.0 | 0.4 | 0 | 0.0 | 0.0 |
| Long range (\|i-j\|≥5) | 368 | 21.8 | 80 | 21.7 | 4.7 | 9 | 2.4 | 0.5 |
| Backbone-Backbone | 40 | 2.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 148 | 8.8 | 45 | 30.4 | 2.7 | 9 | 6.1 | 0.5 |
| Sidechain-Sidechain | 180 | 10.7 | 35 | 19.4 | 2.1 | 0 | 0.0 | 0.0 |
| Inter-chain | 183 | 10.8 | 85 | 46.4 | 5.0 | 10 | 5.5 | 0.6 |
| Backbone-Backbone | 6 | 0.4 | 1 | 16.7 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 43 | 2.5 | 17 | 39.5 | 1.0 | 4 | 9.3 | 0.2 |
| Sidechain-Sidechain | 134 | 7.9 | 67 | 50.0 | 4.0 | 6 | 4.5 | 0.4 |
| 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 | 1687 | 100.0 | 304 | 18.0 | 18.0 | 23 | 1.4 | 1.4 |
| Backbone-Backbone | 150 | 8.9 | 14 | 9.3 | 0.8 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 910 | 53.9 | 143 | 15.7 | 8.5 | 15 | 1.6 | 0.9 |
| Sidechain-Sidechain | 627 | 37.2 | 147 | 23.4 | 8.7 | 8 | 1.3 | 0.5 |

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

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




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

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

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 1 | 17 | 11 | 1 | 24 | 38 | 91 | 0.51 | 2.63 | 0.58 | 0.26 |
| 2 | 12 | 19 | 3 | 24 | 45 | 103 | 0.72 | 3.22 | 0.78 | 0.32 |
| 3 | 11 | 19 | 1 | 23 | 45 | 99 | 0.66 | 3.83 | 0.79 | 0.29 |
| 4 | 19 | 24 | 2 | 24 | 45 | 114 | 0.61 | 3.36 | 0.69 | 0.31 |
| 5 | 25 | 20 | 1 | 26 | 51 | 123 | 0.78 | 4.35 | 1.03 | 0.3 |
| 6 | 21 | 19 | 1 | 33 | 39 | 113 | 0.52 | 2.89 | 0.58 | 0.28 |
| 7 | 14 | 16 | 6 | 24 | 45 | 105 | 0.46 | 3.06 | 0.54 | 0.26 |
| 8 | 21 | 13 | 4 | 21 | 43 | 102 | 0.61 | 3.51 | 0.75 | 0.27 |
| 9 | 14 | 20 | 1 | 24 | 47 | 106 | 0.64 | 3.23 | 0.72 | 0.3 |
| 10 | 11 | 17 | 4 | 21 | 37 | 90 | 0.58 | 3.21 | 0.69 | 0.29 |
| 11 | 17 | 16 | 4 | 31 | 39 | 107 | 0.51 | 3.27 | 0.63 | 0.29 |

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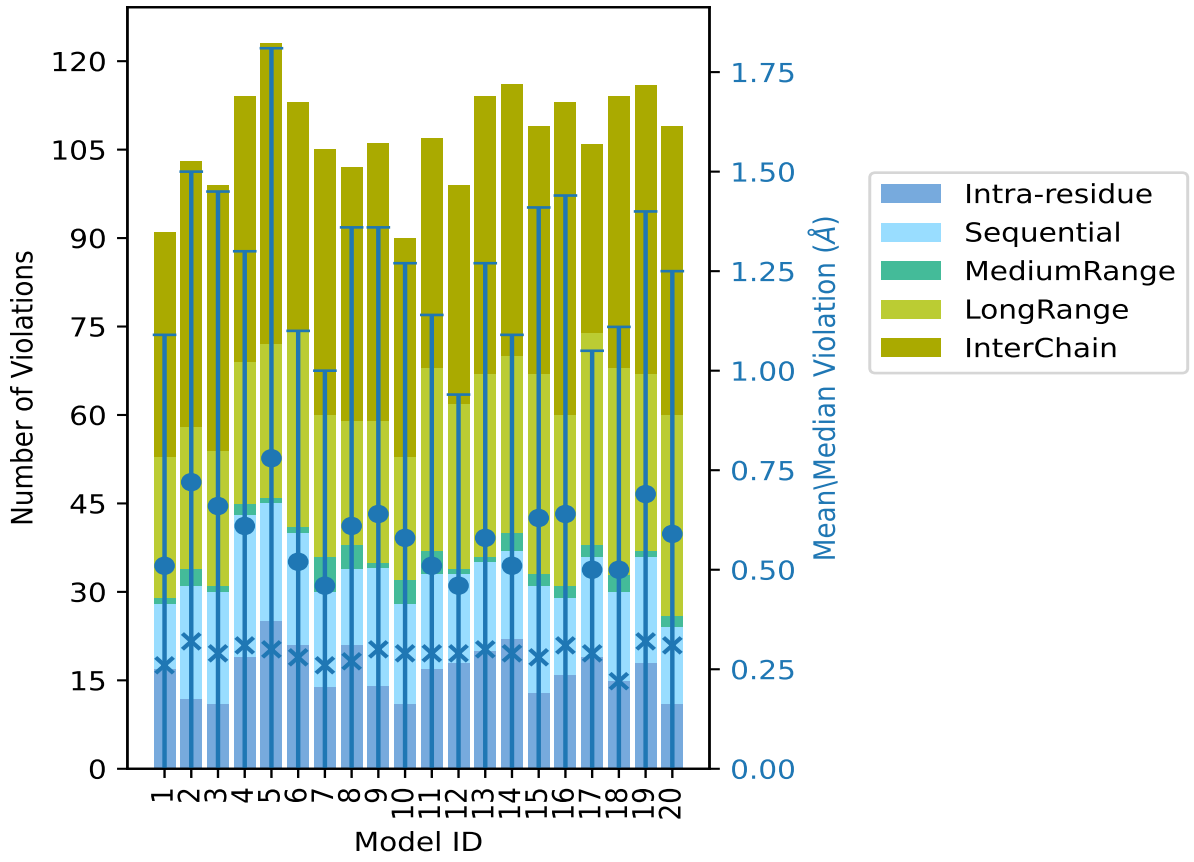
| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 12 | 18 | 15 | 1 | 28 | 37 | 99 | 0.46 | 2.27 | 0.48 | 0.29 |
| 13 | 20 | 15 | 1 | 31 | 47 | 114 | 0.58 | 3.93 | 0.69 | 0.3 |
| 14 | 22 | 15 | 3 | 30 | 46 | 116 | 0.51 | 3.1 | 0.58 | 0.29 |
| 15 | 13 | 18 | 2 | 34 | 42 | 109 | 0.63 | 4.13 | 0.78 | 0.28 |
| 16 | 16 | 13 | 2 | 29 | 53 | 113 | 0.64 | 4.31 | 0.8 | 0.31 |
| 17 | 19 | 17 | 2 | 36 | 32 | 106 | 0.5 | 2.83 | 0.55 | 0.29 |
| 18 | 15 | 15 | 3 | 35 | 46 | 114 | 0.5 | 2.98 | 0.61 | 0.22 |
| 19 | 18 | 18 | 1 | 30 | 49 | 116 | 0.69 | 2.86 | 0.71 | 0.32 |
| 20 | 11 | 13 | 2 | 34 | 49 | 109 | 0.59 | 3.36 | 0.66 | 0.31 |

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

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




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

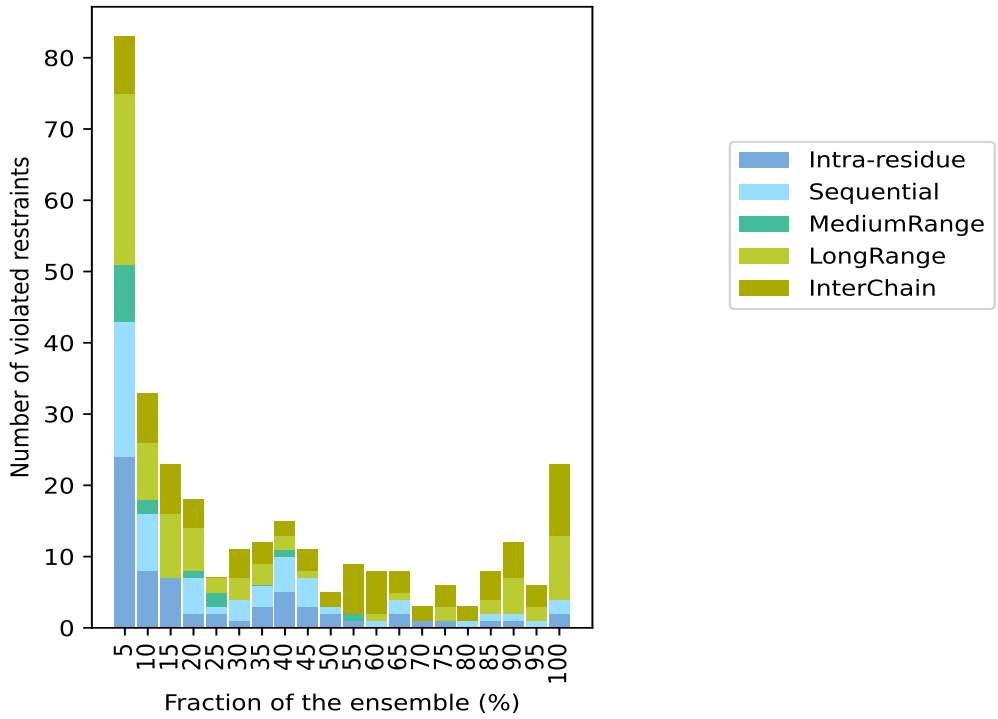
## 9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1383(IR:494, SQ:321, MR:182, LR:288, IC:98) 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] | % |
| 24 | 19 | 8 | 24 | 8 | 83 | 1 | 5.0 |
| 8 | 8 | 2 | 8 | 7 | 33 | 2 | 10.0 |
| 7 | 0 | 0 | 9 | 7 | 23 | 3 | 15.0 |
| 2 | 5 | 1 | 6 | 4 | 18 | 4 | 20.0 |
| 2 | 1 | 2 | 2 | 0 | 7 | 5 | 25.0 |
| 1 | 3 | 0 | 3 | 4 | 11 | 6 | 30.0 |
| 3 | 3 | 0 | 3 | 3 | 12 | 7 | 35.0 |
| 5 | 5 | 1 | 2 | 2 | 15 | 8 | 40.0 |
| 3 | 4 | 0 | 1 | 3 | 11 | 9 | 45.0 |
| 2 | 1 | 0 | 0 | 2 | 5 | 10 | 50.0 |
| 1 | 0 | 1 | 0 | 7 | 9 | 11 | 55.0 |
| 0 | 1 | 0 | 1 | 6 | 8 | 12 | 60.0 |
| 2 | 2 | 0 | 1 | 3 | 8 | 13 | 65.0 |
| 1 | 0 | 0 | 0 | 2 | 3 | 14 | 70.0 |
| 1 | 0 | 0 | 2 | 3 | 6 | 15 | 75.0 |
| 0 | 1 | 0 | 0 | 2 | 3 | 16 | 80.0 |
| 1 | 1 | 0 | 2 | 4 | 8 | 17 | 85.0 |
| 1 | 1 | 0 | 5 | 5 | 12 | 18 | 90.0 |
| 0 | 1 | 0 | 2 | 3 | 6 | 19 | 95.0 |
| 2 | 2 | 0 | 9 | 10 | 23 | 20 | 100.0 |

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

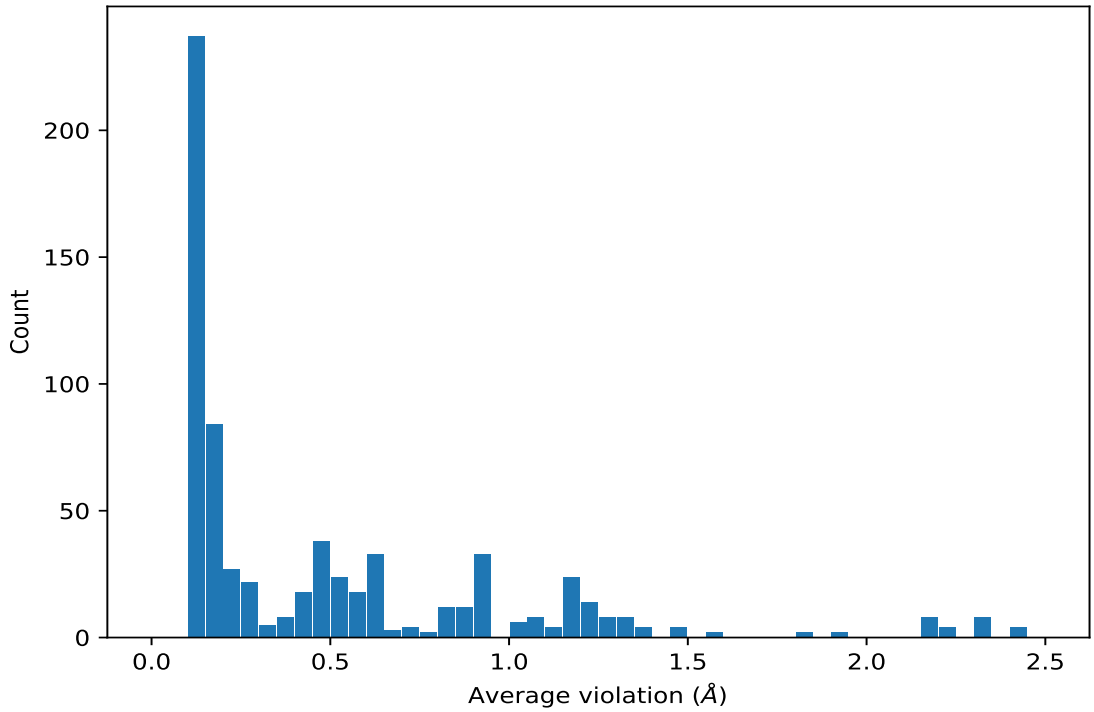
### 9.3.1 Bar graph : Distance violation statistics for the ensemble (i)




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

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

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




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

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

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 20 | 2.24 | 0.69 | 2.16 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 20 | 2.24 | 0.69 | 2.16 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 20 | 2.24 | 0.69 | 2.16 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 20 | 2.24 | 0.69 | 2.16 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 20 | 2.16 | 0.58 | 2.18 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 20 | 2.16 | 0.58 | 2.18 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 20 | 2.16 | 0.58 | 2.18 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 20 | 2.16 | 0.58 | 2.18 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 20 | 2.16 | 0.58 | 2.18 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 20 | 2.16 | 0.58 | 2.18 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 20 | 1.82 | 1.03 | 2.15 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 20 | 1.82 | 1.03 | 2.15 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 20 | 1.48 | 0.97 | 1.18 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 20 | 1.48 | 0.97 | 1.18 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 20 | 1.36 | 0.44 | 1.36 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 20 | 1.36 | 0.44 | 1.36 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 20 | 1.33 | 0.72 | 1.16 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 20 | 1.33 | 0.72 | 1.16 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 20 | 1.33 | 0.72 | 1.16 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 20 | 1.33 | 0.72 | 1.16 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 20 | 1.31 | 0.58 | 1.36 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 20 | 1.31 | 0.58 | 1.36 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 20 | 1.31 | 0.58 | 1.36 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 20 | 1.31 | 0.58 | 1.36 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 20 | 1.2 | 0.42 | 1.08 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 20 | 1.2 | 0.42 | 1.08 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 20 | 1.02 | 0.5 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 20 | 1.02 | 0.5 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 20 | 1.02 | 0.5 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 20 | 1.02 | 0.5 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 20 | 1.02 | 0.5 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 20 | 1.02 | 0.5 | 1.1 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 20 | 0.33 | 0.04 | 0.33 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 20 | 0.32 | 0.04 | 0.32 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 20 | 0.32 | 0.07 | 0.34 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 20 | 0.31 | 0.05 | 0.31 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 20 | 0.31 | 0.05 | 0.32 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 20 | 0.29 | 0.07 | 0.29 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 20 | 0.29 | 0.05 | 0.29 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 20 | 0.28 | 0.05 | 0.28 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 20 | 0.26 | 0.04 | 0.26 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 20 | 0.25 | 0.05 | 0.24 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 20 | 0.24 | 0.05 | 0.24 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 20 | 0.23 | 0.04 | 0.24 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 20 | 0.15 | 0.02 | 0.15 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 20 | 0.15 | 0.02 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 20 | 0.14 | 0.02 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 20 | 0.14 | 0.02 | 0.15 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 19 | 2.43 | 0.91 | 2.08 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 19 | 2.43 | 0.91 | 2.08 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 19 | 2.43 | 0.91 | 2.08 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 19 | 2.43 | 0.91 | 2.08 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 19 | 2.34 | 0.66 | 2.4 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 19 | 2.34 | 0.66 | 2.4 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 19 | 2.33 | 0.83 | 2.14 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 19 | 2.33 | 0.83 | 2.14 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 19 | 2.33 | 0.83 | 2.14 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 19 | 2.33 | 0.83 | 2.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 19 | 2.33 | 0.83 | 2.14 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 19 | 2.33 | 0.83 | 2.14 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 19 | 0.53 | 0.25 | 0.51 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 19 | 0.53 | 0.25 | 0.51 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 19 | 0.27 | 0.07 | 0.31 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 19 | 0.26 | 0.06 | 0.27 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 18 | 2.17 | 0.91 | 2.14 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 18 | 2.17 | 0.91 | 2.14 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD2 | 18 | 1.2 | 0.55 | 1.14 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HE2 | 18 | 1.2 | 0.55 | 1.14 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD1 | 18 | 1.2 | 0.55 | 1.14 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HE1 | 18 | 1.2 | 0.55 | 1.14 |
| (1,139) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HD2 | 18 | 1.2 | 0.55 | 1.14 |
| (1,139) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HD1 | 18 | 1.2 | 0.55 | 1.14 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 18 | 0.95 | 0.56 | 0.85 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 18 | 0.95 | 0.56 | 0.85 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 18 | 0.95 | 0.56 | 0.85 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 18 | 0.95 | 0.56 | 0.85 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 18 | 0.95 | 0.56 | 0.85 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 18 | 0.95 | 0.56 | 0.85 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 18 | 0.82 | 0.59 | 0.6 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 18 | 0.82 | 0.59 | 0.6 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 18 | 0.82 | 0.59 | 0.6 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 18 | 0.82 | 0.59 | 0.6 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 18 | 0.82 | 0.59 | 0.6 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 18 | 0.82 | 0.59 | 0.6 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 18 | 0.55 | 0.22 | 0.68 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 18 | 0.55 | 0.22 | 0.68 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 18 | 0.37 | 0.12 | 0.38 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 18 | 0.37 | 0.12 | 0.38 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 18 | 0.37 | 0.12 | 0.38 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 18 | 0.37 | 0.12 | 0.38 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 18 | 0.28 | 0.06 | 0.27 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 18 | 0.27 | 0.09 | 0.3 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 18 | 0.26 | 0.08 | 0.26 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 18 | 0.26 | 0.07 | 0.27 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 18 | 0.25 | 0.07 | 0.26 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 18 | 0.24 | 0.05 | 0.25 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 17 | 1.91 | 1.07 | 1.74 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 17 | 1.91 | 1.07 | 1.74 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 17 | 1.47 | 0.78 | 1.5 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 17 | 1.47 | 0.78 | 1.5 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 17 | 1.2 | 0.76 | 1.24 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 17 | 1.2 | 0.76 | 1.24 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 17 | 1.2 | 0.76 | 1.24 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 17 | 1.2 | 0.76 | 1.24 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 17 | 1.2 | 0.76 | 1.24 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 17 | 1.2 | 0.76 | 1.24 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 17 | 1.19 | 0.68 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 17 | 1.19 | 0.68 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 17 | 1.19 | 0.68 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 17 | 1.19 | 0.68 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 17 | 1.19 | 0.68 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 17 | 1.19 | 0.68 | 1.09 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 17 | 0.65 | 0.09 | 0.68 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 17 | 0.64 | 0.31 | 0.55 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 17 | 0.64 | 0.31 | 0.55 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 17 | 0.58 | 0.13 | 0.62 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 17 | 0.4 | 0.15 | 0.39 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 17 | 0.4 | 0.15 | 0.39 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 16 | 1.28 | 0.41 | 1.38 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 16 | 1.28 | 0.41 | 1.38 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 16 | 1.28 | 0.41 | 1.38 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 16 | 1.28 | 0.41 | 1.38 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 16 | 1.28 | 0.41 | 1.38 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 16 | 1.28 | 0.41 | 1.38 |
| (1,754) | 2:107:B:TYS:HD1 | 1:223:C:VAL:HG22 | 16 | 1.13 | 0.63 | 1.06 |
| (1,754) | 2:107:B:TYS:HE2 | 1:223:C:VAL:HG22 | 16 | 1.13 | 0.63 | 1.06 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 16 | 1.13 | 0.63 | 1.06 |
| (1,754) | 2:107:B:TYS:HE1 | 1:223:C:VAL:HG22 | 16 | 1.13 | 0.63 | 1.06 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 16 | 0.4 | 0.11 | 0.4 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 16 | 0.4 | 0.11 | 0.4 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 16 | 0.4 | 0.11 | 0.4 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 16 | 0.4 | 0.11 | 0.4 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 15 | 1.21 | 0.99 | 1.24 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 15 | 1.21 | 0.99 | 1.24 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 15 | 1.21 | 0.99 | 1.24 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 15 | 1.21 | 0.99 | 1.24 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 15 | 1.21 | 0.99 | 1.24 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 15 | 1.21 | 0.99 | 1.24 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 15 | 0.58 | 0.41 | 0.53 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 15 | 0.58 | 0.41 | 0.53 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 15 | 0.37 | 0.12 | 0.37 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 15 | 0.37 | 0.12 | 0.37 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 15 | 0.25 | 0.07 | 0.26 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 15 | 0.24 | 0.06 | 0.23 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 15 | 0.16 | 0.04 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 15 | 0.16 | 0.04 | 0.15 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 14 | 1.22 | 0.67 | 1.0 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 14 | 1.22 | 0.67 | 1.0 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 14 | 1.22 | 0.67 | 1.0 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 14 | 1.22 | 0.67 | 1.0 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 14 | 1.22 | 0.67 | 1.0 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 14 | 1.22 | 0.67 | 1.0 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 14 | 0.41 | 0.21 | 0.38 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 14 | 0.41 | 0.21 | 0.38 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 14 | 0.41 | 0.21 | 0.38 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 14 | 0.41 | 0.21 | 0.38 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 14 | 0.41 | 0.21 | 0.38 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 14 | 0.41 | 0.21 | 0.38 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 14 | 0.11 | 0.01 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 14 | 0.11 | 0.01 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 14 | 0.11 | 0.01 | 0.11 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 13 | 1.05 | 0.69 | 0.71 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 13 | 1.05 | 0.69 | 0.71 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 13 | 1.05 | 0.69 | 0.71 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 13 | 1.05 | 0.69 | 0.71 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 13 | 0.52 | 0.33 | 0.4 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 13 | 0.52 | 0.33 | 0.4 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 13 | 0.52 | 0.33 | 0.4 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 13 | 0.51 | 0.17 | 0.54 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 13 | 0.51 | 0.17 | 0.54 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 13 | 0.46 | 0.23 | 0.42 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 13 | 0.46 | 0.23 | 0.42 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 13 | 0.46 | 0.23 | 0.42 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 13 | 0.46 | 0.23 | 0.42 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 13 | 0.46 | 0.23 | 0.42 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 13 | 0.46 | 0.23 | 0.42 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 13 | 0.28 | 0.11 | 0.32 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 13 | 0.28 | 0.11 | 0.32 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 13 | 0.19 | 0.06 | 0.18 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 13 | 0.16 | 0.02 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 13 | 0.16 | 0.02 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 13 | 0.16 | 0.02 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 13 | 0.16 | 0.02 | 0.15 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 13 | 0.11 | 0.01 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 13 | 0.11 | 0.01 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 13 | 0.11 | 0.01 | 0.11 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 12 | 1.07 | 0.78 | 0.74 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 12 | 1.07 | 0.78 | 0.74 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 12 | 1.07 | 0.78 | 0.74 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 12 | 1.07 | 0.78 | 0.74 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 12 | 0.95 | 0.54 | 0.8 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 12 | 0.95 | 0.54 | 0.8 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE1 | 12 | 0.93 | 0.63 | 0.75 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HD2 | 12 | 0.93 | 0.63 | 0.75 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE2 | 12 | 0.93 | 0.63 | 0.75 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 12 | 0.61 | 0.36 | 0.54 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 12 | 0.61 | 0.36 | 0.54 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 12 | 0.58 | 0.21 | 0.62 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 12 | 0.58 | 0.21 | 0.62 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE1 | 12 | 0.49 | 0.42 | 0.31 |
| (1,421) | 1:49:A:VAL:HG13 | 2:121:B:TYS:HE1 | 12 | 0.49 | 0.42 | 0.31 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HD1 | 12 | 0.49 | 0.42 | 0.31 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE2 | 12 | 0.49 | 0.42 | 0.31 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 12 | 0.29 | 0.14 | 0.31 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 12 | 0.22 | 0.06 | 0.22 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 11 | 1.2 | 0.89 | 0.75 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 11 | 1.2 | 0.89 | 0.75 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 11 | 1.2 | 0.89 | 0.75 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 11 | 1.2 | 0.89 | 0.75 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD1 | 11 | 0.92 | 0.76 | 0.68 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD2 | 11 | 0.92 | 0.76 | 0.68 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HE2 | 11 | 0.92 | 0.76 | 0.68 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HE1 | 11 | 0.92 | 0.76 | 0.68 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 11 | 0.9 | 0.56 | 0.72 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 11 | 0.9 | 0.56 | 0.72 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 11 | 0.86 | 0.44 | 0.71 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 11 | 0.86 | 0.44 | 0.71 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 11 | 0.86 | 0.44 | 0.71 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 11 | 0.86 | 0.44 | 0.71 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 11 | 0.16 | 0.02 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 11 | 0.16 | 0.02 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 11 | 0.16 | 0.02 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 11 | 0.16 | 0.02 | 0.15 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 11 | 0.16 | 0.05 | 0.15 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 11 | 0.16 | 0.05 | 0.15 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 11 | 0.15 | 0.01 | 0.15 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 11 | 0.15 | 0.01 | 0.15 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 11 | 0.15 | 0.01 | 0.15 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 11 | 0.14 | 0.02 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 11 | 0.14 | 0.02 | 0.14 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 11 | 0.14 | 0.02 | 0.14 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 11 | 0.14 | 0.02 | 0.14 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 11 | 0.14 | 0.02 | 0.14 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 11 | 0.14 | 0.02 | 0.14 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 11 | 0.12 | 0.02 | 0.12 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 11 | 0.12 | 0.02 | 0.12 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 10 | 0.85 | 0.63 | 0.64 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 10 | 0.85 | 0.63 | 0.64 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 10 | 0.85 | 0.63 | 0.64 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 10 | 0.85 | 0.63 | 0.64 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 10 | 0.85 | 0.63 | 0.64 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 10 | 0.85 | 0.63 | 0.64 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 10 | 0.71 | 0.7 | 0.41 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 10 | 0.71 | 0.7 | 0.41 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 10 | 0.71 | 0.7 | 0.41 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 10 | 0.71 | 0.7 | 0.41 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 10 | 0.7 | 0.03 | 0.7 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 10 | 0.7 | 0.03 | 0.7 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 10 | 0.27 | 0.06 | 0.3 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 10 | 0.27 | 0.06 | 0.3 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 10 | 0.11 | 0.01 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 10 | 0.11 | 0.01 | 0.11 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 9 | 0.63 | 0.44 | 0.62 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 9 | 0.63 | 0.44 | 0.62 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 9 | 0.63 | 0.44 | 0.62 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 9 | 0.63 | 0.57 | 0.43 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 9 | 0.63 | 0.57 | 0.43 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 9 | 0.63 | 0.57 | 0.43 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 9 | 0.63 | 0.57 | 0.43 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 9 | 0.63 | 0.57 | 0.43 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 9 | 0.63 | 0.57 | 0.43 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 9 | 0.42 | 0.18 | 0.43 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 9 | 0.42 | 0.18 | 0.43 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 9 | 0.42 | 0.18 | 0.43 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 9 | 0.42 | 0.18 | 0.43 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 9 | 0.42 | 0.18 | 0.43 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 9 | 0.42 | 0.18 | 0.43 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 9 | 0.28 | 0.08 | 0.3 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 9 | 0.19 | 0.04 | 0.2 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 9 | 0.17 | 0.03 | 0.17 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 9 | 0.17 | 0.03 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 9 | 0.17 | 0.03 | 0.17 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 9 | 0.17 | 0.03 | 0.17 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 9 | 0.17 | 0.03 | 0.18 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 9 | 0.15 | 0.05 | 0.12 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 9 | 0.13 | 0.02 | 0.13 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 9 | 0.12 | 0.02 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 9 | 0.12 | 0.02 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 9 | 0.12 | 0.02 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 9 | 0.12 | 0.02 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 9 | 0.12 | 0.02 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 9 | 0.12 | 0.02 | 0.12 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 9 | 0.12 | 0.01 | 0.11 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 9 | 0.12 | 0.01 | 0.11 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 8 | 0.88 | 0.63 | 0.7 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 8 | 0.88 | 0.63 | 0.7 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 8 | 0.88 | 0.63 | 0.7 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 8 | 0.88 | 0.63 | 0.7 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 8 | 0.88 | 0.63 | 0.7 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 8 | 0.88 | 0.63 | 0.7 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 8 | 0.76 | 0.6 | 0.5 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 8 | 0.76 | 0.6 | 0.5 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 8 | 0.63 | 0.33 | 0.55 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 8 | 0.63 | 0.33 | 0.55 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 8 | 0.63 | 0.33 | 0.55 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 8 | 0.63 | 0.33 | 0.55 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 8 | 0.29 | 0.06 | 0.3 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 8 | 0.24 | 0.04 | 0.25 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 8 | 0.24 | 0.04 | 0.25 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 8 | 0.21 | 0.04 | 0.22 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 8 | 0.21 | 0.04 | 0.22 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 8 | 0.18 | 0.04 | 0.18 |
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 8 | 0.17 | 0.06 | 0.16 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 8 | 0.17 | 0.04 | 0.18 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 8 | 0.15 | 0.03 | 0.15 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 8 | 0.15 | 0.03 | 0.15 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 8 | 0.14 | 0.05 | 0.12 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 8 | 0.14 | 0.05 | 0.12 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 8 | 0.14 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 8 | 0.14 | 0.03 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 8 | 0.14 | 0.03 | 0.15 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 8 | 0.13 | 0.02 | 0.14 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 8 | 0.13 | 0.01 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 8 | 0.13 | 0.01 | 0.13 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 8 | 0.12 | 0.02 | 0.12 |
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 8 | 0.12 | 0.02 | 0.12 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD1 | 7 | 1.23 | 0.44 | 1.31 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD2 | 7 | 1.23 | 0.44 | 1.31 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE1 | 7 | 0.92 | 0.73 | 0.52 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE2 | 7 | 0.92 | 0.73 | 0.52 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE1 | 7 | 0.92 | 0.73 | 0.52 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE2 | 7 | 0.92 | 0.73 | 0.52 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE1 | 7 | 0.92 | 0.73 | 0.52 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE2 | 7 | 0.92 | 0.73 | 0.52 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HD1 | 7 | 0.6 | 0.47 | 0.34 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HE2 | 7 | 0.6 | 0.47 | 0.34 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HE1 | 7 | 0.6 | 0.47 | 0.34 |
| (1,1238) | 1:249:C:VAL:HG13 | 2:321:D:TYS:HE1 | 7 | 0.6 | 0.47 | 0.34 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE1 | 7 | 0.45 | 0.16 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE2 | 7 | 0.45 | 0.16 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE1 | 7 | 0.45 | 0.16 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE2 | 7 | 0.45 | 0.16 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE1 | 7 | 0.45 | 0.16 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE2 | 7 | 0.45 | 0.16 | 0.51 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG21 | 7 | 0.22 | 0.03 | 0.22 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG22 | 7 | 0.22 | 0.03 | 0.22 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG23 | 7 | 0.22 | 0.03 | 0.22 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG21 | 7 | 0.21 | 0.02 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG22 | 7 | 0.21 | 0.02 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG23 | 7 | 0.21 | 0.02 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD2 | 7 | 0.16 | 0.03 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD3 | 7 | 0.16 | 0.03 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD2 | 7 | 0.16 | 0.03 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD3 | 7 | 0.16 | 0.03 | 0.15 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD2 | 7 | 0.14 | 0.05 | 0.13 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD3 | 7 | 0.14 | 0.05 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,699) | 1:67:A:ASN:HA | 1:68:A:LYS:H | 7 | 0.13 | 0.02 | 0.13 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 7 | 0.13 | 0.02 | 0.12 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 7 | 0.13 | 0.01 | 0.12 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 7 | 0.13 | 0.01 | 0.12 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE2 | 7 | 0.13 | 0.01 | 0.12 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE3 | 7 | 0.13 | 0.01 | 0.12 |
| (2,2) | 1:9:A:CYS:CB | 1:34:A:CYS:SG | 7 | 0.12 | 0.01 | 0.11 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE1 | 6 | 1.58 | 0.81 | 1.46 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE2 | 6 | 1.58 | 0.81 | 1.46 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD1 | 6 | 0.89 | 0.42 | 1.06 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD2 | 6 | 0.89 | 0.42 | 1.06 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD1 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD2 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD1 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD2 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD1 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD2 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD1 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD2 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD1 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD2 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD1 | 6 | 0.64 | 0.46 | 0.5 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD2 | 6 | 0.64 | 0.46 | 0.5 |
| (1,1507) | 2:306:D:ILE:HD11 | 2:307:D:TYS:H | 6 | 0.59 | 0.22 | 0.64 |
| (1,1507) | 2:306:D:ILE:HD12 | 2:307:D:TYS:H | 6 | 0.59 | 0.22 | 0.64 |
| (1,1507) | 2:306:D:ILE:HD13 | 2:307:D:TYS:H | 6 | 0.59 | 0.22 | 0.64 |
| (1,1504) | 2:306:D:ILE:HB | 2:307:D:TYS:H | 6 | 0.26 | 0.03 | 0.26 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE2 | 6 | 0.18 | 0.03 | 0.18 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE3 | 6 | 0.18 | 0.03 | 0.18 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE1 | 6 | 0.18 | 0.11 | 0.11 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE2 | 6 | 0.18 | 0.11 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE1 | 6 | 0.18 | 0.11 | 0.11 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE2 | 6 | 0.18 | 0.11 | 0.11 |
| (3,16) | 1:28:A:ILE:O | 1:226:C:LEU:N | 6 | 0.16 | 0.04 | 0.16 |
| (1,1035) | 1:224:C:LYS:HG2 | 1:225:C:HIS:H | 6 | 0.13 | 0.02 | 0.12 |
| (1,1035) | 1:224:C:LYS:HG3 | 1:225:C:HIS:H | 6 | 0.13 | 0.02 | 0.12 |
| (1,1130) | 1:237:C:GLN:H | 1:253:C:PRO:HG3 | 6 | 0.13 | 0.02 | 0.12 |
| (2,14) | 1:209:C:CYS:CB | 1:234:C:CYS:SG | 6 | 0.12 | 0.01 | 0.12 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD2 | 5 | 0.24 | 0.05 | 0.27 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD3 | 5 | 0.24 | 0.05 | 0.27 |
| (3,29) | 1:227:C:LYS:H | 1:239:C:VAL:O | 5 | 0.18 | 0.04 | 0.17 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG2 | 5 | 0.16 | 0.02 | 0.17 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG3 | 5 | 0.16 | 0.02 | 0.17 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG2 | 5 | 0.15 | 0.03 | 0.15 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG3 | 5 | 0.15 | 0.03 | 0.15 |
| (1,1446) | 1:264:C:LYS:HG3 | 1:265:C:CYS:H | 5 | 0.14 | 0.02 | 0.14 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD2 | 5 | 0.13 | 0.01 | 0.13 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD3 | 5 | 0.13 | 0.01 | 0.13 |
| (2,17) | 1:211:C:CYS:CB | 1:250:C:CYS:SG | 5 | 0.11 | 0.01 | 0.11 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE1 | 4 | 0.56 | 0.32 | 0.55 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE2 | 4 | 0.56 | 0.32 | 0.55 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD1 | 4 | 0.5 | 0.21 | 0.44 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD2 | 4 | 0.5 | 0.21 | 0.44 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD1 | 4 | 0.5 | 0.21 | 0.44 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD2 | 4 | 0.5 | 0.21 | 0.44 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD1 | 4 | 0.5 | 0.21 | 0.44 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD2 | 4 | 0.5 | 0.21 | 0.44 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD1 | 4 | 0.46 | 0.16 | 0.46 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD2 | 4 | 0.46 | 0.16 | 0.46 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD1 | 4 | 0.46 | 0.16 | 0.46 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD2 | 4 | 0.46 | 0.16 | 0.46 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD1 | 4 | 0.46 | 0.16 | 0.46 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD2 | 4 | 0.46 | 0.16 | 0.46 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD1 | 4 | 0.24 | 0.21 | 0.14 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD2 | 4 | 0.24 | 0.21 | 0.14 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD1 | 4 | 0.24 | 0.21 | 0.14 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD2 | 4 | 0.24 | 0.21 | 0.14 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD1 | 4 | 0.24 | 0.21 | 0.14 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD2 | 4 | 0.24 | 0.21 | 0.14 |
| (1,655) | 1:64:A:LYS:HG3 | 1:65:A:CYS:H | 4 | 0.17 | 0.04 | 0.16 |
| (1,64) | 1:15:A:GLU:HG2 | 2:123:B:SER:HA | 4 | 0.16 | 0.04 | 0.14 |
| (1,64) | 1:15:A:GLU:HG3 | 2:123:B:SER:HA | 4 | 0.16 | 0.04 | 0.14 |
| (1,935) | 1:215:C:GLU:HG2 | 2:323:D:SER:HA | 4 | 0.15 | 0.04 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,935) | 1:215:C:GLU:HG3 | 2:323:D:SER:HA | 4 | 0.15 | 0.04 | 0.14 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG11 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG12 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG13 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG21 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG22 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG23 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG11 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG12 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG13 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG21 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG22 | 4 | 0.15 | 0.03 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG23 | 4 | 0.15 | 0.03 | 0.16 |
| (3,15) | 1:28:A:ILE:O | 1:226:C:LEU:H | 4 | 0.14 | 0.03 | 0.15 |
| (1,69) | 1:16:A:SER:HB2 | 1:52:A:ASP:H | 4 | 0.14 | 0.03 | 0.15 |
| (1,69) | 1:16:A:SER:HB3 | 1:52:A:ASP:H | 4 | 0.14 | 0.03 | 0.15 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE3 | 4 | 0.14 | 0.01 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE2 | 4 | 0.14 | 0.01 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE3 | 4 | 0.14 | 0.01 | 0.14 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB2 | 4 | 0.13 | 0.03 | 0.13 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB3 | 4 | 0.13 | 0.03 | 0.13 |
| (1,940) | 1:216:C:SER:HB2 | 1:252:C:ASP:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,940) | 1:216:C:SER:HB3 | 1:252:C:ASP:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE1 | 4 | 0.12 | 0.03 | 0.11 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE2 | 4 | 0.12 | 0.03 | 0.11 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE1 | 4 | 0.12 | 0.03 | 0.11 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE2 | 4 | 0.12 | 0.03 | 0.11 |
| (2,5) | 1:11:A:CYS:CB | 1:50:A:CYS:SG | 4 | 0.11 | 0.0 | 0.11 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG2 | 4 | 0.11 | 0.02 | 0.1 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG3 | 4 | 0.11 | 0.02 | 0.1 |
| (1,248) | 1:27:A:LYS:HE2 | 1:225:C:HIS:HE1 | 4 | 0.11 | 0.01 | 0.11 |
| (1,248) | 1:27:A:LYS:HE3 | 1:225:C:HIS:HE1 | 4 | 0.11 | 0.01 | 0.11 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD11 | 4 | 0.11 | 0.01 | 0.11 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD12 | 4 | 0.11 | 0.01 | 0.11 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD13 | 4 | 0.11 | 0.01 | 0.11 |
| (1,15) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HD1 | 3 | 1.26 | 0.37 | 1.07 |
| (1,15) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HD2 | 3 | 1.26 | 0.37 | 1.07 |
| (1,889) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HD1 | 3 | 0.58 | 0.42 | 0.29 |
| (1,889) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HD2 | 3 | 0.58 | 0.42 | 0.29 |
| (1,86) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HD1 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HD2 | 3 | 0.45 | 0.29 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,86) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HD1 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HD2 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HD1 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HD2 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HD1 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HD2 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HD1 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HD2 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HD1 | 3 | 0.45 | 0.29 | 0.26 |
| (1,86) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HD2 | 3 | 0.45 | 0.29 | 0.26 |
| (2,1) | 1:9:A:CYS:CB | 1:34:A:CYS:CB | 3 | 0.37 | 0.29 | 0.23 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD11 | 3 | 0.19 | 0.1 | 0.12 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD12 | 3 | 0.19 | 0.1 | 0.12 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD13 | 3 | 0.19 | 0.1 | 0.12 |
| (1,1516) | 2:307:D:TYS:H | 2:307:D:TYS:HB3 | 3 | 0.19 | 0.08 | 0.16 |
| (1,1516) | 2:307:D:TYS:H | 2:307:D:TYS:HB3 | 3 | 0.19 | 0.08 | 0.16 |
| (1,843) | 2:130:B:ARG:H | 2:130:B:ARG:HG2 | 3 | 0.18 | 0.07 | 0.14 |
| (1,843) | 2:130:B:ARG:H | 2:130:B:ARG:HG3 | 3 | 0.18 | 0.07 | 0.14 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG21 | 3 | 0.17 | 0.03 | 0.18 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG22 | 3 | 0.17 | 0.03 | 0.18 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG23 | 3 | 0.17 | 0.03 | 0.18 |
| (1,483) | 1:54:A:LYS:HB3 | 1:54:A:LYS:HE2 | 3 | 0.16 | 0.04 | 0.15 |
| (1,483) | 1:54:A:LYS:HB3 | 1:54:A:LYS:HE3 | 3 | 0.16 | 0.04 | 0.15 |
| (3,6) | 1:26:A:LEU:N | 1:228:C:ILE:O | 3 | 0.15 | 0.02 | 0.15 |
| (1,691) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HB2 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HB3 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HB2 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HB3 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HB2 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HB3 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HB2 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HB3 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HB2 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HB3 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HB2 | 3 | 0.15 | 0.02 | 0.14 |
| (1,691) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HB3 | 3 | 0.15 | 0.02 | 0.14 |
| (1,648) | 1:64:A:LYS:HB3 | 1:64:A:LYS:HE2 | 3 | 0.14 | 0.03 | 0.13 |
| (1,648) | 1:64:A:LYS:HB3 | 1:64:A:LYS:HE3 | 3 | 0.14 | 0.03 | 0.13 |
| (1,1263) | 1:251:C:ILE:HG21 | 1:258:C:ILE:HG12 | 3 | 0.14 | 0.0 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG21 | 1:258:C:ILE:HG13 | 3 | 0.14 | 0.0 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG22 | 1:258:C:ILE:HG12 | 3 | 0.14 | 0.0 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG22 | 1:258:C:ILE:HG13 | 3 | 0.14 | 0.0 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1263) | 1:251:C:ILE:HG23 | 1:258:C:ILE:HG12 | 3 | 0.14 | 0.0 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG23 | 1:258:C:ILE:HG13 | 3 | 0.14 | 0.0 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD11 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD12 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD13 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD21 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD22 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD23 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD11 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD12 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD13 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD21 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD22 | 3 | 0.13 | 0.01 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD23 | 3 | 0.13 | 0.01 | 0.14 |
| (1,182) | 1:25:A:HIS:HE1 | 1:227:C:LYS:HE2 | 3 | 0.13 | 0.01 | 0.13 |
| (1,182) | 1:25:A:HIS:HE1 | 1:227:C:LYS:HE3 | 3 | 0.13 | 0.01 | 0.13 |
| (1,92) | 1:18:A:VAL:HG11 | 1:23:A:VAL:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,92) | 1:18:A:VAL:HG12 | 1:23:A:VAL:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,92) | 1:18:A:VAL:HG13 | 1:23:A:VAL:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,92) | 1:18:A:VAL:HG21 | 1:23:A:VAL:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,92) | 1:18:A:VAL:HG22 | 1:23:A:VAL:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,92) | 1:18:A:VAL:HG23 | 1:23:A:VAL:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,136) | 1:23:A:VAL:HB | 1:42:A:LEU:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,1157) | 1:238:C:ILE:HG21 | 1:251:C:ILE:HB | 3 | 0.12 | 0.01 | 0.12 |
| (1,1157) | 1:238:C:ILE:HG22 | 1:251:C:ILE:HB | 3 | 0.12 | 0.01 | 0.12 |
| (1,1157) | 1:238:C:ILE:HG23 | 1:251:C:ILE:HB | 3 | 0.12 | 0.01 | 0.12 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD11 | 3 | 0.12 | 0.01 | 0.11 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD12 | 3 | 0.12 | 0.01 | 0.11 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD13 | 3 | 0.12 | 0.01 | 0.11 |
| (1,773) | 2:114:B:GLU:H | 2:114:B:GLU:HG2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,773) | 2:114:B:GLU:H | 2:114:B:GLU:HG3 | 3 | 0.11 | 0.0 | 0.11 |
| (1,779) | 2:115:B:GLU:HA | 2:115:B:GLU:HG2 | 3 | 0.11 | 0.0 | 0.11 |
| (1,779) | 2:115:B:GLU:HA | 2:115:B:GLU:HG3 | 3 | 0.11 | 0.0 | 0.11 |
| (2,6) | 1:11:A:CYS:SG | 1:50:A:CYS:CB | 3 | 0.11 | 0.0 | 0.11 |
| (2,18) | 1:211:C:CYS:SG | 1:250:C:CYS:CB | 3 | 0.1 | 0.0 | 0.1 |
| (1,10) | 1:10:A:PRO:HA | 2:112:B:TYS:HD1 | 2 | 1.39 | 0.28 | 1.39 |
| (1,10) | 1:10:A:PRO:HA | 2:112:B:TYS:HD2 | 2 | 1.39 | 0.28 | 1.39 |
| (1,1558) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 2 | 0.64 | 0.34 | 0.64 |
| (1,1558) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 2 | 0.64 | 0.34 | 0.64 |
| (1,1558) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HD1 | 2 | 0.64 | 0.34 | 0.64 |
| (1,1558) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HD2 | 2 | 0.64 | 0.34 | 0.64 |
| (1,881) | 1:210:C:PRO:HA | 2:312:D:TYS:HD1 | 2 | 0.52 | 0.09 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,881) | 1:210:C:PRO:HA | 2:312:D:TYS:HD2 | 2 | 0.52 | 0.09 | 0.52 |
| (1,23) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HD1 | 2 | 0.49 | 0.22 | 0.49 |
| (1,23) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HD2 | 2 | 0.49 | 0.22 | 0.49 |
| (1,23) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HD1 | 2 | 0.49 | 0.22 | 0.49 |
| (1,23) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HD2 | 2 | 0.49 | 0.22 | 0.49 |
| (2,13) | 1:209:C:CYS:CB | 1:234:C:CYS:CB | 2 | 0.39 | 0.28 | 0.39 |
| (1,1502) | 2:306:D:ILE:HA | 2:307:D:TYS:H | 2 | 0.3 | 0.02 | 0.3 |
| (1,113) | 1:20:A:ARG:HD2 | 1:23:A:VAL:H | 2 | 0.2 | 0.07 | 0.2 |
| (1,113) | 1:20:A:ARG:HD3 | 1:23:A:VAL:H | 2 | 0.2 | 0.07 | 0.2 |
| (1,809) | 2:125:B:LYS:H | 2:125:B:LYS:HG2 | 2 | 0.2 | 0.08 | 0.2 |
| (1,809) | 2:125:B:LYS:H | 2:125:B:LYS:HG3 | 2 | 0.2 | 0.08 | 0.2 |
| (1,1573) | 2:325:D:LYS:H | 2:325:D:LYS:HG2 | 2 | 0.17 | 0.06 | 0.17 |
| (1,1573) | 2:325:D:LYS:H | 2:325:D:LYS:HG3 | 2 | 0.17 | 0.06 | 0.17 |
| (1,167) | 1:24:A:LYS:HG2 | 1:43:A:LYS:H | 2 | 0.16 | 0.04 | 0.16 |
| (1,167) | 1:24:A:LYS:HG3 | 1:43:A:LYS:H | 2 | 0.16 | 0.04 | 0.16 |
| (1,447) | 1:51:A:ILE:HG21 | 1:58:A:ILE:HG12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,447) | 1:51:A:ILE:HG21 | 1:58:A:ILE:HG13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,447) | 1:51:A:ILE:HG22 | 1:58:A:ILE:HG12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,447) | 1:51:A:ILE:HG22 | 1:58:A:ILE:HG13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,447) | 1:51:A:ILE:HG23 | 1:58:A:ILE:HG12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,447) | 1:51:A:ILE:HG23 | 1:58:A:ILE:HG13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,681) | 1:66:A:LEU:HD21 | 1:263:C:GLU:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,681) | 1:66:A:LEU:HD22 | 1:263:C:GLU:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,681) | 1:66:A:LEU:HD23 | 1:263:C:GLU:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,961) | 1:218:C:VAL:HG11 | 1:252:C:ASP:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,961) | 1:218:C:VAL:HG12 | 1:252:C:ASP:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,961) | 1:218:C:VAL:HG13 | 1:252:C:ASP:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,961) | 1:218:C:VAL:HG21 | 1:252:C:ASP:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,961) | 1:218:C:VAL:HG22 | 1:252:C:ASP:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,961) | 1:218:C:VAL:HG23 | 1:252:C:ASP:H | 2 | 0.14 | 0.03 | 0.14 |
| (1,862) | 2:132:B:GLU:H | 2:132:B:GLU:HG2 | 2 | 0.14 | 0.0 | 0.14 |
| (1,862) | 2:132:B:GLU:H | 2:132:B:GLU:HG3 | 2 | 0.14 | 0.0 | 0.14 |
| (1,295) | 1:29:A:LEU:HD21 | 1:225:C:HIS:HE1 | 2 | 0.14 | 0.01 | 0.14 |
| (1,295) | 1:29:A:LEU:HD22 | 1:225:C:HIS:HE1 | 2 | 0.14 | 0.01 | 0.14 |
| (1,295) | 1:29:A:LEU:HD23 | 1:225:C:HIS:HE1 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1443) | 1:264:C:LYS:HG2 | 1:265:C:CYS:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,799) | 2:121:B:TYS:HA | 2:121:B:TYS:HD1 | 2 | 0.13 | 0.02 | 0.13 |
| (1,799) | 2:121:B:TYS:HA | 2:121:B:TYS:HD2 | 2 | 0.13 | 0.02 | 0.13 |
| (1,830) | 2:127:B:PRO:HG2 | 2:128:B:ALA:H | 2 | 0.13 | 0.0 | 0.13 |
| (1,830) | 2:127:B:PRO:HG3 | 2:128:B:ALA:H | 2 | 0.13 | 0.0 | 0.13 |
| (1,960) | 1:218:C:VAL:HG11 | 1:223:C:VAL:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,960) | 1:218:C:VAL:HG12 | 1:223:C:VAL:H | 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) |
|---|---|---|---|---|---|---|
| (1,960) | 1:218:C:VAL:HG13 | 1:223:C:VAL:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,960) | 1:218:C:VAL:HG21 | 1:223:C:VAL:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,960) | 1:218:C:VAL:HG22 | 1:223:C:VAL:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,960) | 1:218:C:VAL:HG23 | 1:223:C:VAL:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,1045) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1045) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,1603) | 2:330:D:ARG:H | 2:330:D:ARG:HG2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1603) | 2:330:D:ARG:H | 2:330:D:ARG:HG3 | 2 | 0.12 | 0.02 | 0.12 |
| (3,5) | 1:26:A:LEU:H | 1:228:C:ILE:O | 2 | 0.12 | 0.02 | 0.12 |
| (1,187) | 1:25:A:HIS:HE1 | 1:41:A:ARG:HG2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,187) | 1:25:A:HIS:HE1 | 1:41:A:ARG:HG3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,341) | 1:38:A:ILE:HG21 | 1:51:A:ILE:HB | 2 | 0.12 | 0.0 | 0.12 |
| (1,341) | 1:38:A:ILE:HG22 | 1:51:A:ILE:HB | 2 | 0.12 | 0.0 | 0.12 |
| (1,341) | 1:38:A:ILE:HG23 | 1:51:A:ILE:HB | 2 | 0.12 | 0.0 | 0.12 |
| (1,903) | 1:212:C:ARG:HD2 | 1:213:C:PHE:HE1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,903) | 1:212:C:ARG:HD2 | 1:213:C:PHE:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,903) | 1:212:C:ARG:HD3 | 1:213:C:PHE:HE1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,903) | 1:212:C:ARG:HD3 | 1:213:C:PHE:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1533) | 2:313:D:THR:HA | 2:314:D:GLU:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,291) | 1:29:A:LEU:HD11 | 1:225:C:HIS:HE1 | 2 | 0.11 | 0.0 | 0.11 |
| (1,291) | 1:29:A:LEU:HD12 | 1:225:C:HIS:HE1 | 2 | 0.11 | 0.0 | 0.11 |
| (1,291) | 1:29:A:LEU:HD13 | 1:225:C:HIS:HE1 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG11 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG12 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG13 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG23 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG11 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG12 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG13 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG23 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1543) | 2:315:D:GLU:HA | 2:315:D:GLU:HG2 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1543) | 2:315:D:GLU:HA | 2:315:D:GLU:HG3 | 2 | 0.11 | 0.01 | 0.11 |
| (1,828) | 2:127:B:PRO:HD2 | 2:128:B:ALA:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,828) | 2:127:B:PRO:HD3 | 2:128:B:ALA:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,868) | 2:138:B:LYS:HA | 2:138:B:LYS:HE2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,868) | 2:138:B:LYS:HA | 2:138:B:LYS:HE3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1592) | 2:327:D:PRO:HG2 | 2:328:D:ALA:H | 2 | 0.1 | 0.0 | 0.1 |
| (1,1592) | 2:327:D:PRO:HG3 | 2:328:D:ALA:H | 2 | 0.1 | 0.0 | 0.1 |

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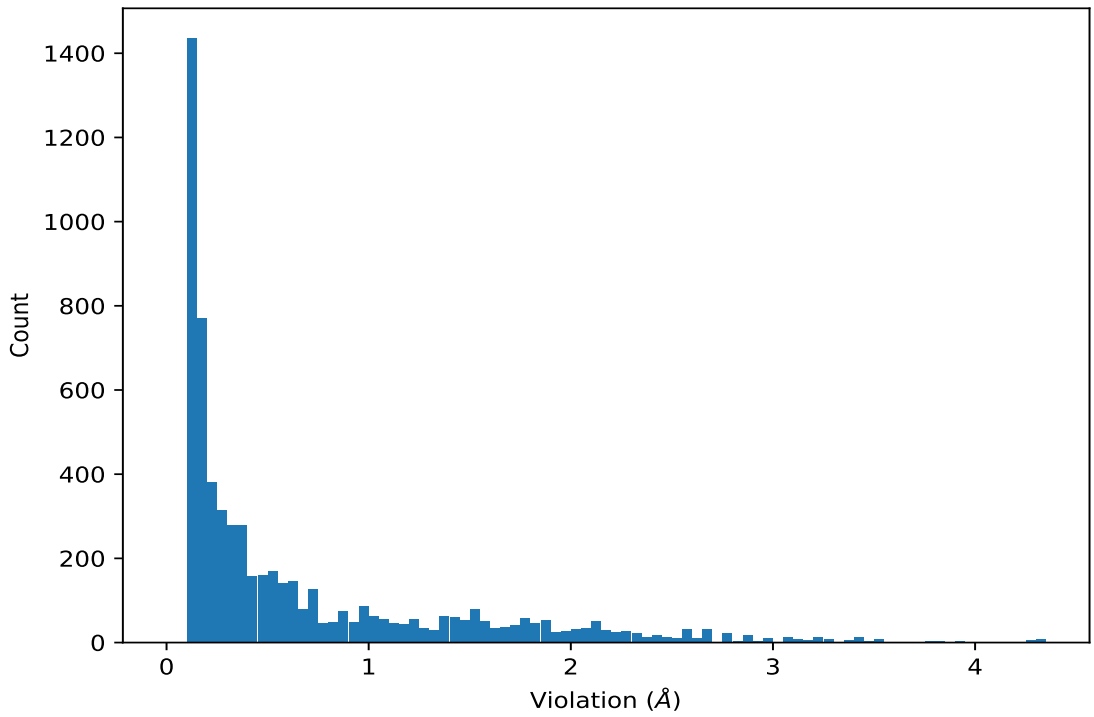
| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,1623) | 2:332:D:GLU:HA | 2:332:D:GLU:HG2 | 2 | 0.1 | 0.0 | 0.1 |
| (1,1623) | 2:332:D:GLU:HA | 2:332:D:GLU:HG3 | 2 | 0.1 | 0.0 | 0.1 |

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

## 9.5 All violated distance restraints (i)

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

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




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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 5 | 4.35 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 5 | 4.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 5 | 4.35 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 5 | 4.35 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 16 | 4.31 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 16 | 4.31 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 16 | 4.31 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 16 | 4.31 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 5 | 4.27 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 5 | 4.27 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 5 | 4.27 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 5 | 4.27 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 5 | 4.27 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 5 | 4.27 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 15 | 4.13 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 15 | 4.13 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 13 | 3.93 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 13 | 3.93 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 5 | 3.92 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 5 | 3.92 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 3 | 3.83 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 3 | 3.83 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 3 | 3.83 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 3 | 3.83 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 5 | 3.75 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 5 | 3.75 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 5 | 3.75 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 5 | 3.75 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 16 | 3.52 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 16 | 3.52 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 8 | 3.51 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 8 | 3.51 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 8 | 3.51 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 8 | 3.51 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 8 | 3.51 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 8 | 3.51 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 5 | 3.45 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 5 | 3.45 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 5 | 3.45 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 5 | 3.45 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 15 | 3.41 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 15 | 3.41 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 15 | 3.41 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 15 | 3.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 15 | 3.41 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 15 | 3.41 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 13 | 3.4 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 13 | 3.4 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 13 | 3.4 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 13 | 3.4 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 13 | 3.4 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 13 | 3.4 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 3 | 3.39 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 3 | 3.39 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 20 | 3.36 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 20 | 3.36 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 4 | 3.36 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 4 | 3.36 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 16 | 3.3 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 16 | 3.3 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 11 | 3.27 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 11 | 3.27 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 5 | 3.25 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 5 | 3.25 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 5 | 3.25 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 5 | 3.25 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 5 | 3.25 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 5 | 3.25 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 9 | 3.23 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 9 | 3.23 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 9 | 3.23 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 9 | 3.23 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 9 | 3.23 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 9 | 3.23 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 2 | 3.22 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 2 | 3.22 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 10 | 3.21 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 10 | 3.21 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 5 | 3.21 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 5 | 3.21 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 9 | 3.19 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 9 | 3.19 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 11 | 3.15 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 11 | 3.15 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 11 | 3.15 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 11 | 3.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 5 | 3.14 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 5 | 3.14 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 5 | 3.14 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 5 | 3.14 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 5 | 3.14 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 5 | 3.14 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 14 | 3.1 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 14 | 3.1 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 16 | 3.09 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 16 | 3.09 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 16 | 3.09 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 16 | 3.09 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 16 | 3.09 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 16 | 3.09 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 7 | 3.06 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 7 | 3.06 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 10 | 3.05 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 10 | 3.05 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 10 | 3.05 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 10 | 3.05 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 2 | 2.99 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 2 | 2.99 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 2 | 2.99 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 2 | 2.99 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 8 | 2.99 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 8 | 2.99 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 18 | 2.98 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 18 | 2.98 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE1 | 5 | 2.98 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE2 | 5 | 2.98 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 9 | 2.93 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 9 | 2.93 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 9 | 2.93 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 9 | 2.93 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 6 | 2.89 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 6 | 2.89 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 5 | 2.88 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 5 | 2.88 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 5 | 2.88 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 5 | 2.88 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 15 | 2.88 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 15 | 2.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 4 | 2.87 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 4 | 2.87 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 4 | 2.87 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 4 | 2.87 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 19 | 2.86 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 19 | 2.86 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 19 | 2.86 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 19 | 2.86 |
| (1,139) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HD2 | 9 | 2.85 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 17 | 2.83 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 17 | 2.83 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 5 | 2.81 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 5 | 2.81 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD2 | 15 | 2.79 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 2 | 2.79 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 2 | 2.79 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 2 | 2.79 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 2 | 2.79 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 15 | 2.78 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 15 | 2.78 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 15 | 2.78 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 15 | 2.78 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 2 | 2.76 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 2 | 2.76 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 2 | 2.76 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 2 | 2.76 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 2 | 2.76 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 2 | 2.76 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 20 | 2.75 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 20 | 2.75 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 20 | 2.75 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 20 | 2.75 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 20 | 2.75 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 20 | 2.75 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 5 | 2.75 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 5 | 2.75 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 3 | 2.74 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 3 | 2.74 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 18 | 2.69 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 18 | 2.69 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 18 | 2.69 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 18 | 2.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 13 | 2.69 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 13 | 2.69 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 20 | 2.69 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 20 | 2.69 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 20 | 2.69 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 20 | 2.69 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 8 | 2.68 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 2 | 2.68 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 2 | 2.68 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 2 | 2.66 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 2 | 2.66 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 2 | 2.66 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 2 | 2.66 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 2 | 2.66 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 2 | 2.66 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 19 | 2.66 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 19 | 2.66 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 19 | 2.66 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 19 | 2.66 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 19 | 2.66 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 19 | 2.66 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 20 | 2.65 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 20 | 2.65 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 20 | 2.65 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 20 | 2.65 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 20 | 2.65 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 20 | 2.65 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 1 | 2.63 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 1 | 2.63 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 5 | 2.63 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 5 | 2.63 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 5 | 2.63 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 5 | 2.63 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 15 | 2.6 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 15 | 2.6 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 15 | 2.6 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 15 | 2.6 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 18 | 2.59 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 18 | 2.59 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 1 | 2.59 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 1 | 2.59 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 1 | 2.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 1 | 2.59 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 1 | 2.59 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 1 | 2.59 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 16 | 2.59 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 16 | 2.59 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 16 | 2.59 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 16 | 2.59 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 16 | 2.59 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 16 | 2.59 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 16 | 2.58 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 16 | 2.58 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 16 | 2.58 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 16 | 2.58 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 16 | 2.58 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 16 | 2.58 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 9 | 2.57 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 9 | 2.57 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 14 | 2.57 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 14 | 2.57 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 14 | 2.57 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 14 | 2.57 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 14 | 2.57 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 14 | 2.57 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 3 | 2.56 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 3 | 2.56 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 3 | 2.56 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 3 | 2.56 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 16 | 2.54 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 16 | 2.54 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 16 | 2.54 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 16 | 2.54 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 8 | 2.53 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 8 | 2.53 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 8 | 2.53 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 8 | 2.53 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HD2 | 5 | 2.53 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 18 | 2.52 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 18 | 2.52 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 4 | 2.49 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 4 | 2.49 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 2 | 2.49 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 2 | 2.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 14 | 2.48 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 14 | 2.48 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 14 | 2.48 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 14 | 2.48 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 4 | 2.45 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 4 | 2.45 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 4 | 2.45 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 4 | 2.45 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 4 | 2.45 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 4 | 2.45 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 15 | 2.44 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 15 | 2.44 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 7 | 2.43 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 7 | 2.43 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 3 | 2.41 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 3 | 2.41 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 3 | 2.41 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 3 | 2.41 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 3 | 2.41 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 3 | 2.41 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 10 | 2.4 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 10 | 2.4 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 10 | 2.4 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 10 | 2.4 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 13 | 2.4 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 13 | 2.4 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 19 | 2.4 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 19 | 2.4 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 14 | 2.39 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 14 | 2.39 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 19 | 2.39 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 19 | 2.39 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 10 | 2.39 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 10 | 2.39 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 6 | 2.37 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 6 | 2.37 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 8 | 2.37 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 8 | 2.37 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 8 | 2.37 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 8 | 2.37 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 11 | 2.36 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 11 | 2.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 10 | 2.33 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 10 | 2.33 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 10 | 2.33 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 10 | 2.33 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 10 | 2.33 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 10 | 2.33 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 3 | 2.33 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 3 | 2.33 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 2 | 2.33 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 2 | 2.33 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 2 | 2.33 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 2 | 2.33 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 2 | 2.33 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 2 | 2.33 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 2 | 2.33 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 2 | 2.33 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 2 | 2.32 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 2 | 2.32 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 4 | 2.32 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 4 | 2.32 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 19 | 2.31 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 19 | 2.31 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 12 | 2.27 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 12 | 2.27 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 12 | 2.27 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 12 | 2.27 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 4 | 2.27 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 4 | 2.27 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 8 | 2.26 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 8 | 2.26 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 8 | 2.26 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 8 | 2.26 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 8 | 2.26 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 8 | 2.26 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 4 | 2.26 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 4 | 2.26 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 4 | 2.26 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 4 | 2.26 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 4 | 2.26 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 4 | 2.26 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 1 | 2.26 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 1 | 2.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 1 | 2.26 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 1 | 2.26 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 7 | 2.25 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 7 | 2.25 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 7 | 2.25 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 7 | 2.25 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 7 | 2.25 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 7 | 2.25 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 19 | 2.24 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 19 | 2.24 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 19 | 2.24 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 19 | 2.24 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 19 | 2.24 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 19 | 2.24 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 3 | 2.24 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 3 | 2.24 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 3 | 2.24 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 3 | 2.24 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 16 | 2.22 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 16 | 2.22 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 16 | 2.22 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 16 | 2.22 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 16 | 2.22 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 16 | 2.22 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 6 | 2.21 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 6 | 2.21 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 6 | 2.21 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 6 | 2.21 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 6 | 2.21 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 6 | 2.21 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 16 | 2.21 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 16 | 2.21 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 8 | 2.19 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 8 | 2.19 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 8 | 2.19 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 8 | 2.19 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 19 | 2.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 19 | 2.19 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 19 | 2.19 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE1 | 13 | 2.19 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE2 | 13 | 2.19 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 2 | 2.18 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 2 | 2.18 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 17 | 2.16 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 17 | 2.16 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 17 | 2.16 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 17 | 2.16 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 17 | 2.16 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 17 | 2.16 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 11 | 2.16 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 11 | 2.16 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 11 | 2.16 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 11 | 2.16 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 14 | 2.14 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 14 | 2.14 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 14 | 2.14 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 14 | 2.14 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 14 | 2.14 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 14 | 2.14 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 3 | 2.14 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 3 | 2.14 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 3 | 2.14 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 3 | 2.14 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 3 | 2.14 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 3 | 2.14 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 8 | 2.14 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 8 | 2.14 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 8 | 2.14 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 8 | 2.14 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 8 | 2.14 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 8 | 2.14 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 4 | 2.14 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 4 | 2.14 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 12 | 2.14 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 12 | 2.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 20 | 2.13 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 20 | 2.13 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 13 | 2.12 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 13 | 2.12 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 13 | 2.12 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 13 | 2.12 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 5 | 2.12 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 5 | 2.12 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 5 | 2.12 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 5 | 2.12 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 5 | 2.12 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 5 | 2.12 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 19 | 2.11 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 19 | 2.11 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 20 | 2.11 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 20 | 2.11 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 20 | 2.11 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 20 | 2.11 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 5 | 2.1 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 5 | 2.1 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 5 | 2.1 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 5 | 2.1 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 11 | 2.1 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 11 | 2.1 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 11 | 2.1 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 11 | 2.1 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 11 | 2.1 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 11 | 2.1 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 6 | 2.09 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 6 | 2.09 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 6 | 2.09 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 6 | 2.09 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 6 | 2.09 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 6 | 2.09 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 19 | 2.09 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 19 | 2.09 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 12 | 2.09 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 12 | 2.09 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 4 | 2.08 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 4 | 2.08 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 4 | 2.08 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 4 | 2.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 4 | 2.08 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 4 | 2.08 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 5 | 2.08 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 5 | 2.08 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 5 | 2.08 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 5 | 2.08 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 5 | 2.08 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 5 | 2.08 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 9 | 2.08 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 9 | 2.08 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 9 | 2.08 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 9 | 2.08 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 17 | 2.07 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 17 | 2.07 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 17 | 2.07 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 17 | 2.07 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 17 | 2.07 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 17 | 2.07 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 8 | 2.07 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 8 | 2.07 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 19 | 2.06 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE1 | 5 | 2.04 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE2 | 5 | 2.04 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE1 | 5 | 2.04 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE2 | 5 | 2.04 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE1 | 5 | 2.04 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE2 | 5 | 2.04 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 6 | 2.04 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 6 | 2.04 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 6 | 2.04 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 6 | 2.04 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 10 | 2.04 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 10 | 2.04 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 10 | 2.04 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 10 | 2.04 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 11 | 2.02 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 11 | 2.02 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 11 | 2.02 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 11 | 2.02 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 11 | 2.02 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 11 | 2.02 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 13 | 2.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 13 | 2.01 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 13 | 2.01 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 13 | 2.01 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 15 | 2.0 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 15 | 2.0 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 3 | 2.0 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 3 | 2.0 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 3 | 2.0 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 3 | 2.0 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 3 | 2.0 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 3 | 2.0 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 4 | 1.99 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 4 | 1.99 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 4 | 1.99 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 4 | 1.99 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 16 | 1.99 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 16 | 1.99 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 16 | 1.99 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 16 | 1.99 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 9 | 1.98 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 9 | 1.98 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 9 | 1.98 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 9 | 1.98 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 13 | 1.98 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 13 | 1.98 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 13 | 1.98 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 13 | 1.98 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 6 | 1.96 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 6 | 1.96 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 6 | 1.96 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 6 | 1.96 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 6 | 1.96 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 6 | 1.96 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 13 | 1.96 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 13 | 1.96 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 13 | 1.96 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 13 | 1.96 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 13 | 1.96 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 13 | 1.96 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 7 | 1.94 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 7 | 1.94 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 7 | 1.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 7 | 1.94 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 14 | 1.94 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 14 | 1.94 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD2 | 19 | 1.94 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 19 | 1.93 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 19 | 1.93 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 19 | 1.93 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 19 | 1.93 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 3 | 1.9 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 3 | 1.9 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 3 | 1.9 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 3 | 1.9 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 3 | 1.9 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 3 | 1.9 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 10 | 1.9 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 10 | 1.9 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 10 | 1.9 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 10 | 1.9 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 10 | 1.9 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 10 | 1.9 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 3 | 1.9 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 3 | 1.9 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 19 | 1.89 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 19 | 1.89 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 19 | 1.89 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 19 | 1.89 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 19 | 1.89 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 19 | 1.89 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 5 | 1.89 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 5 | 1.89 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 5 | 1.89 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 5 | 1.89 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 5 | 1.89 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 5 | 1.89 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 7 | 1.89 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 7 | 1.89 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 8 | 1.87 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 8 | 1.87 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 8 | 1.87 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 8 | 1.87 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 8 | 1.87 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 8 | 1.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 1 | 1.87 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 1 | 1.87 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 1 | 1.87 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 1 | 1.87 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 1 | 1.87 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 1 | 1.87 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 20 | 1.87 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 20 | 1.87 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 20 | 1.87 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 20 | 1.87 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 20 | 1.87 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 20 | 1.87 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 11 | 1.87 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 11 | 1.87 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 11 | 1.87 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 11 | 1.87 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 8 | 1.87 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 8 | 1.87 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 8 | 1.87 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 8 | 1.87 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 8 | 1.87 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 8 | 1.87 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD1 | 19 | 1.87 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 4 | 1.86 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 4 | 1.86 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 4 | 1.86 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 4 | 1.86 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 4 | 1.86 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 4 | 1.86 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 3 | 1.85 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 3 | 1.85 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 8 | 1.85 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 8 | 1.85 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 5 | 1.84 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 5 | 1.84 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 5 | 1.84 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 5 | 1.84 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 17 | 1.84 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 17 | 1.84 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 13 | 1.83 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 13 | 1.83 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 5 | 1.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 5 | 1.83 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 5 | 1.83 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 5 | 1.83 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 5 | 1.83 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 5 | 1.83 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 13 | 1.82 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 13 | 1.82 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 13 | 1.82 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 13 | 1.82 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 13 | 1.82 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 13 | 1.82 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 14 | 1.82 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 14 | 1.82 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 14 | 1.82 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 14 | 1.82 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 16 | 1.81 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 16 | 1.81 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 17 | 1.81 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 17 | 1.81 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 17 | 1.81 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 17 | 1.81 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD1 | 8 | 1.81 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 17 | 1.8 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 17 | 1.8 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 17 | 1.8 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 17 | 1.8 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 17 | 1.8 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 17 | 1.8 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 20 | 1.8 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 20 | 1.8 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 20 | 1.8 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 20 | 1.8 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 18 | 1.8 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 18 | 1.8 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 18 | 1.8 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 18 | 1.8 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD1 | 4 | 1.8 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD2 | 4 | 1.8 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 3 | 1.79 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 3 | 1.79 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 3 | 1.79 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 3 | 1.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 2 | 1.79 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 2 | 1.79 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 18 | 1.78 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 18 | 1.78 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE1 | 15 | 1.78 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE2 | 15 | 1.78 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE1 | 15 | 1.78 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE2 | 15 | 1.78 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE1 | 15 | 1.78 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE2 | 15 | 1.78 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 11 | 1.78 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 11 | 1.78 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 11 | 1.78 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 11 | 1.78 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 11 | 1.78 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 11 | 1.78 |
| (1,15) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HD1 | 9 | 1.78 |
| (1,15) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HD2 | 9 | 1.78 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 15 | 1.78 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 15 | 1.78 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 6 | 1.77 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 6 | 1.77 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 6 | 1.77 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 6 | 1.77 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 19 | 1.76 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 19 | 1.76 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 19 | 1.76 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 19 | 1.76 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 3 | 1.76 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 3 | 1.76 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 12 | 1.76 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 12 | 1.76 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 12 | 1.76 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 12 | 1.76 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 12 | 1.76 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 12 | 1.76 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 10 | 1.75 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 10 | 1.75 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 10 | 1.75 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 10 | 1.75 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 10 | 1.75 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 10 | 1.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 18 | 1.75 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 18 | 1.75 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 18 | 1.75 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 18 | 1.75 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 18 | 1.75 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 18 | 1.75 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 10 | 1.75 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 10 | 1.75 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 10 | 1.75 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 10 | 1.75 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 10 | 1.75 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 10 | 1.75 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 2 | 1.74 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 2 | 1.74 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 18 | 1.74 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 18 | 1.74 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 18 | 1.74 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 18 | 1.74 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 18 | 1.74 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 18 | 1.74 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 2 | 1.74 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 2 | 1.74 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 2 | 1.74 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 2 | 1.74 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 2 | 1.74 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 2 | 1.74 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 18 | 1.74 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 18 | 1.74 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 9 | 1.73 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 9 | 1.73 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 6 | 1.72 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 6 | 1.72 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 6 | 1.72 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 6 | 1.72 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 5 | 1.71 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 5 | 1.71 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 5 | 1.71 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 5 | 1.71 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 5 | 1.71 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 5 | 1.71 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 4 | 1.71 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 4 | 1.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 4 | 1.71 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 4 | 1.71 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 4 | 1.71 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 4 | 1.71 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 15 | 1.71 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 15 | 1.71 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 15 | 1.71 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 15 | 1.71 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 15 | 1.71 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 15 | 1.71 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 15 | 1.71 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 1 | 1.69 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 1 | 1.69 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 11 | 1.69 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 11 | 1.69 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 11 | 1.69 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 11 | 1.69 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 11 | 1.69 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 11 | 1.69 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 6 | 1.69 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 6 | 1.69 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 6 | 1.69 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 6 | 1.69 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 17 | 1.69 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 20 | 1.68 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 20 | 1.68 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 9 | 1.68 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 9 | 1.68 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 9 | 1.68 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 9 | 1.68 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 9 | 1.68 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 9 | 1.68 |
| (1,10) | 1:10:A:PRO:HA | 2:112:B:TYS:HD1 | 9 | 1.67 |
| (1,10) | 1:10:A:PRO:HA | 2:112:B:TYS:HD2 | 9 | 1.67 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 6 | 1.66 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 6 | 1.66 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 1 | 1.65 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 1 | 1.65 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 1 | 1.65 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 1 | 1.65 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 1 | 1.65 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 1 | 1.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 18 | 1.65 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 18 | 1.65 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 18 | 1.65 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 18 | 1.65 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 8 | 1.65 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 8 | 1.65 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 7 | 1.64 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 7 | 1.64 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 9 | 1.64 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 9 | 1.64 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 19 | 1.62 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 19 | 1.62 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 7 | 1.61 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 7 | 1.61 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 7 | 1.61 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 7 | 1.61 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 7 | 1.61 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 7 | 1.61 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 10 | 1.61 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 10 | 1.61 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 19 | 1.6 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 19 | 1.6 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 19 | 1.6 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 19 | 1.6 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 19 | 1.6 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 19 | 1.6 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 12 | 1.6 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 12 | 1.6 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 12 | 1.6 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 12 | 1.6 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 12 | 1.6 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 12 | 1.6 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 19 | 1.6 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 19 | 1.6 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 19 | 1.6 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 19 | 1.6 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 4 | 1.6 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 4 | 1.6 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 12 | 1.6 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 12 | 1.6 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 9 | 1.59 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 9 | 1.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 9 | 1.59 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 9 | 1.59 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD1 | 8 | 1.58 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD2 | 8 | 1.58 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 13 | 1.58 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 13 | 1.58 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 13 | 1.58 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 13 | 1.58 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE1 | 16 | 1.58 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE2 | 16 | 1.58 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 17 | 1.57 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 17 | 1.57 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 17 | 1.57 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 17 | 1.57 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 17 | 1.57 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 17 | 1.57 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 8 | 1.57 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 8 | 1.57 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 8 | 1.57 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 8 | 1.57 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 20 | 1.57 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 20 | 1.57 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 20 | 1.57 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 20 | 1.57 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 20 | 1.57 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 20 | 1.57 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 9 | 1.56 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 9 | 1.56 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 9 | 1.56 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 9 | 1.56 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 9 | 1.56 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 9 | 1.56 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 9 | 1.56 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 9 | 1.56 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 9 | 1.56 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 9 | 1.56 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 9 | 1.56 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 9 | 1.56 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 17 | 1.56 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 17 | 1.56 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 17 | 1.56 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 17 | 1.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD1 | 6 | 1.56 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD2 | 6 | 1.56 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 20 | 1.56 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 20 | 1.56 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 20 | 1.56 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 20 | 1.56 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE1 | 9 | 1.55 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 19 | 1.54 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 19 | 1.54 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 19 | 1.54 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD2 | 15 | 1.54 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 16 | 1.52 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 16 | 1.52 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 10 | 1.52 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 10 | 1.52 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 10 | 1.52 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 10 | 1.52 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 10 | 1.52 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 10 | 1.52 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 18 | 1.52 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 18 | 1.52 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 20 | 1.52 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 20 | 1.52 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 16 | 1.52 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 16 | 1.52 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 16 | 1.52 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 16 | 1.52 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 16 | 1.52 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 16 | 1.52 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 2 | 1.51 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 2 | 1.51 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 2 | 1.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 2 | 1.51 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 2 | 1.51 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 2 | 1.51 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 1 | 1.51 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 1 | 1.51 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 1 | 1.51 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 1 | 1.51 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 20 | 1.51 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 20 | 1.51 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 20 | 1.51 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 20 | 1.51 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 19 | 1.51 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 19 | 1.51 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 2 | 1.5 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 2 | 1.5 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 2 | 1.5 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 2 | 1.5 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 2 | 1.5 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 2 | 1.5 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 15 | 1.5 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 15 | 1.5 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 15 | 1.5 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 15 | 1.5 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 9 | 1.5 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 9 | 1.5 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 9 | 1.5 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 9 | 1.5 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 9 | 1.5 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 9 | 1.5 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 1 | 1.5 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 1 | 1.5 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 1 | 1.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 1 | 1.5 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 19 | 1.5 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 19 | 1.5 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 17 | 1.49 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 17 | 1.49 |
| (1,754) | 2:107:B:TYS:HE1 | 1:223:C:VAL:HG22 | 14 | 1.49 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 1 | 1.48 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 1 | 1.48 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 17 | 1.47 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 17 | 1.47 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 17 | 1.47 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 17 | 1.47 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 17 | 1.47 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 17 | 1.47 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 1 | 1.47 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 1 | 1.47 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 1 | 1.47 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 1 | 1.47 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 6 | 1.47 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 6 | 1.47 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 6 | 1.47 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 6 | 1.47 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE1 | 19 | 1.47 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 10 | 1.47 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 10 | 1.47 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 10 | 1.47 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 10 | 1.47 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 10 | 1.47 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 10 | 1.47 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 20 | 1.46 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 20 | 1.46 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 20 | 1.46 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 20 | 1.46 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 20 | 1.46 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 20 | 1.46 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 12 | 1.45 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 12 | 1.45 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 12 | 1.45 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 12 | 1.45 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 12 | 1.45 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 12 | 1.45 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 6 | 1.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 6 | 1.45 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 6 | 1.45 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 6 | 1.45 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 18 | 1.45 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 18 | 1.45 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 18 | 1.45 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 18 | 1.45 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 18 | 1.45 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 18 | 1.45 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 20 | 1.45 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 20 | 1.45 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 20 | 1.45 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 20 | 1.45 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 20 | 1.45 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 20 | 1.45 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 17 | 1.44 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 17 | 1.44 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 17 | 1.44 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 17 | 1.44 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 17 | 1.44 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 17 | 1.44 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD1 | 7 | 1.44 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 5 | 1.43 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 5 | 1.43 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 5 | 1.43 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 5 | 1.43 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 5 | 1.43 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 5 | 1.43 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 14 | 1.43 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 14 | 1.43 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 4 | 1.43 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 4 | 1.43 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 4 | 1.43 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 4 | 1.43 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 4 | 1.43 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 4 | 1.43 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 5 | 1.42 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 5 | 1.42 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 17 | 1.42 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 17 | 1.42 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 3 | 1.41 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 3 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 6 | 1.4 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 6 | 1.4 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 14 | 1.4 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 14 | 1.4 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 14 | 1.4 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 14 | 1.4 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 14 | 1.4 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 14 | 1.4 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD1 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD2 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD1 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD2 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD1 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD2 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD1 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD2 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD1 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD2 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD1 | 19 | 1.4 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD2 | 19 | 1.4 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 3 | 1.4 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 3 | 1.4 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 3 | 1.4 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 3 | 1.4 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 3 | 1.4 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 3 | 1.4 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 9 | 1.4 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 9 | 1.4 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 11 | 1.4 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 11 | 1.4 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 11 | 1.4 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 11 | 1.4 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 11 | 1.4 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 11 | 1.4 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE1 | 17 | 1.38 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE2 | 17 | 1.38 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE1 | 17 | 1.38 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE2 | 17 | 1.38 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE1 | 17 | 1.38 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE2 | 17 | 1.38 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 11 | 1.38 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 11 | 1.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 11 | 1.38 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 11 | 1.38 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 11 | 1.38 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 11 | 1.38 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 16 | 1.38 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 16 | 1.38 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 16 | 1.38 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 16 | 1.38 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 16 | 1.38 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 16 | 1.38 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 15 | 1.37 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 15 | 1.37 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HE1 | 16 | 1.36 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 12 | 1.36 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 12 | 1.36 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 11 | 1.35 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 11 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 15 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 15 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 15 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 15 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 15 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 15 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 16 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 16 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 16 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 16 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 16 | 1.35 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 16 | 1.35 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 12 | 1.35 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 12 | 1.35 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 12 | 1.35 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 12 | 1.35 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 12 | 1.35 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 12 | 1.35 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 19 | 1.35 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 19 | 1.35 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 19 | 1.35 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 19 | 1.35 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 19 | 1.35 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 19 | 1.35 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 16 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 16 | 1.35 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 20 | 1.35 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 20 | 1.35 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 20 | 1.35 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 20 | 1.35 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 20 | 1.35 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 20 | 1.35 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 3 | 1.35 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 3 | 1.35 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 3 | 1.35 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 3 | 1.35 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 3 | 1.35 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 3 | 1.35 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HE2 | 11 | 1.34 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 15 | 1.33 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 15 | 1.33 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 15 | 1.33 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 15 | 1.33 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 15 | 1.33 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 15 | 1.33 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 6 | 1.33 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 6 | 1.33 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE1 | 9 | 1.33 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE2 | 9 | 1.33 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 19 | 1.32 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 19 | 1.32 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD1 | 3 | 1.32 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD2 | 3 | 1.32 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 3 | 1.31 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 3 | 1.31 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD1 | 18 | 1.31 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD2 | 18 | 1.31 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HE1 | 14 | 1.31 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 14 | 1.3 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 14 | 1.3 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 14 | 1.3 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 14 | 1.3 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 11 | 1.3 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 11 | 1.3 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 11 | 1.3 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 11 | 1.3 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 11 | 1.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 11 | 1.3 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 12 | 1.29 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 12 | 1.29 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 12 | 1.29 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 12 | 1.29 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 1 | 1.27 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 1 | 1.27 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 1 | 1.27 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 1 | 1.27 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 15 | 1.27 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 15 | 1.27 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 1 | 1.27 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 1 | 1.27 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 9 | 1.26 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 9 | 1.26 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 19 | 1.26 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 19 | 1.26 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD1 | 2 | 1.26 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD2 | 2 | 1.26 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 17 | 1.25 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 17 | 1.25 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 17 | 1.25 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 17 | 1.25 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HD1 | 9 | 1.25 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HD2 | 13 | 1.25 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 2 | 1.24 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 2 | 1.24 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 2 | 1.24 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 2 | 1.24 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 2 | 1.24 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 2 | 1.24 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 2 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 2 | 1.24 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 2 | 1.24 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 2 | 1.24 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 2 | 1.24 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 2 | 1.24 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE1 | 15 | 1.24 |
| (1,288) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HE2 | 15 | 1.24 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE1 | 15 | 1.24 |
| (1,288) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HE2 | 15 | 1.24 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 4 | 1.24 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 4 | 1.24 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 4 | 1.24 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 4 | 1.24 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD1 | 15 | 1.24 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD2 | 15 | 1.24 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 18 | 1.23 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 18 | 1.23 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 7 | 1.23 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 7 | 1.23 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 11 | 1.23 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 11 | 1.23 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 11 | 1.23 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 11 | 1.23 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 11 | 1.23 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 11 | 1.23 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 20 | 1.23 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 20 | 1.23 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 10 | 1.23 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 10 | 1.23 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 10 | 1.23 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 10 | 1.23 |
| (1,1554) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HD1 | 2 | 1.22 |
| (1,1554) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HD2 | 2 | 1.22 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 14 | 1.21 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 14 | 1.21 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 14 | 1.21 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 14 | 1.21 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 2 | 1.21 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 2 | 1.21 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 2 | 1.21 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 2 | 1.21 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE1 | 19 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 12 | 1.2 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 12 | 1.2 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 10 | 1.2 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 10 | 1.2 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 6 | 1.2 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 6 | 1.2 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 17 | 1.19 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 17 | 1.19 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 3 | 1.19 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 3 | 1.19 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 3 | 1.19 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 3 | 1.19 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 14 | 1.19 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 14 | 1.19 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 14 | 1.19 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 14 | 1.19 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 14 | 1.19 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 14 | 1.19 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 6 | 1.18 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 6 | 1.18 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 6 | 1.18 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 6 | 1.18 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 6 | 1.18 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 6 | 1.18 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 3 | 1.18 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 3 | 1.18 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 3 | 1.18 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 3 | 1.18 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 3 | 1.18 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 3 | 1.18 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 1 | 1.18 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 1 | 1.18 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 1 | 1.18 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 1 | 1.18 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 1 | 1.18 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 1 | 1.18 |
| (1,889) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HD1 | 15 | 1.18 |
| (1,889) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HD2 | 15 | 1.18 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HE1 | 8 | 1.17 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 12 | 1.17 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 12 | 1.17 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD1 | 1 | 1.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 13 | 1.17 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 13 | 1.17 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 14 | 1.16 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 14 | 1.16 |
| (1,754) | 2:107:B:TYS:HD1 | 1:223:C:VAL:HG22 | 1 | 1.16 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD2 | 1 | 1.16 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 20 | 1.16 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 20 | 1.16 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HE2 | 4 | 1.15 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 4 | 1.13 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 4 | 1.13 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 3 | 1.13 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 3 | 1.13 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 3 | 1.13 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 3 | 1.13 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 3 | 1.13 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 3 | 1.13 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD1 | 2 | 1.13 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD2 | 2 | 1.13 |
| (1,754) | 2:107:B:TYS:HD1 | 1:223:C:VAL:HG22 | 18 | 1.13 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 16 | 1.13 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 16 | 1.13 |
| (1,754) | 2:107:B:TYS:HD1 | 1:223:C:VAL:HG22 | 7 | 1.12 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 15 | 1.12 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 15 | 1.12 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 15 | 1.12 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 15 | 1.12 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 15 | 1.12 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 15 | 1.12 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD1 | 5 | 1.12 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 5 | 1.11 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 5 | 1.11 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 5 | 1.11 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 5 | 1.11 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 5 | 1.11 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 5 | 1.11 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 6 | 1.11 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 6 | 1.11 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 6 | 1.11 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 6 | 1.11 |
| (1,10) | 1:10:A:PRO:HA | 2:112:B:TYS:HD1 | 13 | 1.11 |
| (1,10) | 1:10:A:PRO:HA | 2:112:B:TYS:HD2 | 13 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 2 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 2 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 2 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 2 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 2 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 2 | 1.1 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 4 | 1.1 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 4 | 1.1 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 14 | 1.1 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 14 | 1.1 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 14 | 1.1 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 14 | 1.1 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE1 | 14 | 1.1 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 19 | 1.09 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 19 | 1.09 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 19 | 1.09 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 19 | 1.09 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 19 | 1.09 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 19 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 2 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 2 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 2 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 2 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 2 | 1.09 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 2 | 1.09 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 1 | 1.08 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 1 | 1.08 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD1 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD2 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD1 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD2 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD1 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD2 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD1 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD2 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD1 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD2 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD1 | 18 | 1.08 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD2 | 18 | 1.08 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 20 | 1.07 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 20 | 1.07 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 20 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 20 | 1.07 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 20 | 1.07 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 20 | 1.07 |
| (1,15) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HD1 | 13 | 1.07 |
| (1,15) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HD2 | 13 | 1.07 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 9 | 1.06 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 9 | 1.06 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 2 | 1.06 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 2 | 1.06 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 2 | 1.06 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 2 | 1.06 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 10 | 1.06 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 10 | 1.06 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD1 | 13 | 1.06 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 20 | 1.05 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 20 | 1.05 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 9 | 1.04 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 9 | 1.04 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 4 | 1.04 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 4 | 1.04 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 4 | 1.04 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 4 | 1.04 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 4 | 1.04 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 4 | 1.04 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 8 | 1.03 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 8 | 1.03 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD1 | 14 | 1.03 |
| (1,1122) | 1:231:C:THR:HG21 | 2:312:D:TYS:HD2 | 14 | 1.03 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD1 | 14 | 1.03 |
| (1,1122) | 1:231:C:THR:HG22 | 2:312:D:TYS:HD2 | 14 | 1.03 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD1 | 14 | 1.03 |
| (1,1122) | 1:231:C:THR:HG23 | 2:312:D:TYS:HD2 | 14 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 13 | 1.03 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 13 | 1.03 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 13 | 1.03 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 13 | 1.03 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 13 | 1.03 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 13 | 1.03 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 11 | 1.03 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 11 | 1.03 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 11 | 1.03 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 11 | 1.03 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 13 | 1.03 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 13 | 1.03 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 13 | 1.03 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 13 | 1.03 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE1 | 19 | 1.03 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE2 | 19 | 1.03 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 18 | 1.02 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 18 | 1.02 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 18 | 1.02 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 18 | 1.02 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 18 | 1.02 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 18 | 1.02 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE1 | 16 | 1.02 |
| (1,1082) | 1:227:C:LYS:HG2 | 2:312:D:TYS:HE2 | 16 | 1.02 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 7 | 1.02 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 7 | 1.02 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 7 | 1.02 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 7 | 1.02 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 7 | 1.02 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 7 | 1.02 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 6 | 1.01 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 6 | 1.01 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 19 | 1.01 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 19 | 1.01 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 19 | 1.01 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 19 | 1.01 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 19 | 1.01 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 19 | 1.01 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 19 | 1.01 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 19 | 1.01 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 19 | 1.01 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 19 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE1 | 16 | 1.0 |
| (1,1109) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HE2 | 16 | 1.0 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE1 | 16 | 1.0 |
| (1,1109) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HE2 | 16 | 1.0 |
| (1,754) | 2:107:B:TYS:HD1 | 1:223:C:VAL:HG22 | 16 | 1.0 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 10 | 0.98 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 10 | 0.98 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 1 | 0.98 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 1 | 0.98 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 19 | 0.98 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 19 | 0.98 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 19 | 0.98 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 19 | 0.98 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 19 | 0.98 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 19 | 0.98 |
| (1,1558) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 2 | 0.97 |
| (1,1558) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 2 | 0.97 |
| (1,1558) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HD1 | 2 | 0.97 |
| (1,1558) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HD2 | 2 | 0.97 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 14 | 0.97 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 14 | 0.97 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 19 | 0.97 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 19 | 0.97 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 19 | 0.97 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 19 | 0.97 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 19 | 0.97 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 19 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 13 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 13 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 13 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 13 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 13 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 13 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 18 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 18 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 18 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 18 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 18 | 0.97 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 18 | 0.97 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 4 | 0.97 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 4 | 0.97 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 4 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 4 | 0.97 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 4 | 0.97 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 4 | 0.97 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 9 | 0.97 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 9 | 0.97 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD1 | 18 | 0.97 |
| (1,303) | 1:31:A:THR:HG21 | 2:112:B:TYS:HD2 | 18 | 0.97 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD1 | 18 | 0.97 |
| (1,303) | 1:31:A:THR:HG22 | 2:112:B:TYS:HD2 | 18 | 0.97 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD1 | 18 | 0.97 |
| (1,303) | 1:31:A:THR:HG23 | 2:112:B:TYS:HD2 | 18 | 0.97 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 4 | 0.96 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 4 | 0.96 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 16 | 0.96 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 16 | 0.96 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 4 | 0.96 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 4 | 0.96 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 5 | 0.96 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 5 | 0.96 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 5 | 0.96 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 8 | 0.96 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 8 | 0.96 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 8 | 0.96 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 8 | 0.96 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 8 | 0.96 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 8 | 0.96 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 6 | 0.95 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 6 | 0.95 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 6 | 0.95 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 6 | 0.95 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 6 | 0.95 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 6 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 10 | 0.95 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 10 | 0.95 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 15 | 0.95 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 15 | 0.95 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 15 | 0.95 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 4 | 0.95 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 4 | 0.95 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD1 | 16 | 0.95 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HE1 | 7 | 0.94 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 19 | 0.94 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 19 | 0.94 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 19 | 0.94 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 19 | 0.94 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 20 | 0.93 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 20 | 0.93 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 20 | 0.93 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 20 | 0.93 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 20 | 0.93 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 20 | 0.93 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 20 | 0.93 |
| (1,15) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HD1 | 5 | 0.93 |
| (1,15) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HD2 | 5 | 0.93 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 4 | 0.92 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 4 | 0.92 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 11 | 0.92 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 11 | 0.92 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 11 | 0.92 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 11 | 0.92 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 11 | 0.92 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 11 | 0.92 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 15 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 15 | 0.91 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 8 | 0.91 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 8 | 0.91 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 18 | 0.91 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 18 | 0.91 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 13 | 0.9 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 13 | 0.9 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 9 | 0.9 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 9 | 0.9 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 9 | 0.9 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 9 | 0.9 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 9 | 0.9 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 9 | 0.9 |
| (1,754) | 2:107:B:TYS:HD1 | 1:223:C:VAL:HG22 | 5 | 0.9 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 8 | 0.89 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 8 | 0.89 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 8 | 0.89 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 8 | 0.89 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 8 | 0.89 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 8 | 0.89 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 4 | 0.89 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 4 | 0.89 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 4 | 0.89 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 4 | 0.89 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 4 | 0.89 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 4 | 0.89 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 13 | 0.88 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 13 | 0.88 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 13 | 0.88 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 13 | 0.88 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 13 | 0.88 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 13 | 0.88 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 11 | 0.88 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 11 | 0.88 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 10 | 0.88 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 10 | 0.88 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 10 | 0.88 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 10 | 0.88 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD1 | 10 | 0.88 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD2 | 10 | 0.88 |
| (1,1507) | 2:306:D:ILE:HD11 | 2:307:D:TYS:H | 17 | 0.87 |
| (1,1507) | 2:306:D:ILE:HD12 | 2:307:D:TYS:H | 17 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1507) | 2:306:D:ILE:HD13 | 2:307:D:TYS:H | 17 | 0.87 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 8 | 0.87 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 8 | 0.87 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 8 | 0.87 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 8 | 0.87 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 8 | 0.87 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 8 | 0.87 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 13 | 0.87 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 13 | 0.87 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 13 | 0.87 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 13 | 0.87 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 12 | 0.86 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 12 | 0.86 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 14 | 0.86 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 14 | 0.86 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 14 | 0.86 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 14 | 0.86 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 20 | 0.86 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 20 | 0.86 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 3 | 0.86 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 3 | 0.86 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HE2 | 2 | 0.86 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 10 | 0.85 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 10 | 0.85 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 10 | 0.85 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 10 | 0.85 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 10 | 0.85 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 10 | 0.85 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 18 | 0.85 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 18 | 0.85 |
| (1,86) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HD1 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HD2 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HD1 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HD2 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HD1 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HD2 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HD1 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HD2 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HD1 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HD2 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HD1 | 19 | 0.85 |
| (1,86) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HD2 | 19 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 20 | 0.85 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 20 | 0.85 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 20 | 0.85 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 20 | 0.85 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 12 | 0.84 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 12 | 0.84 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD1 | 5 | 0.84 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD2 | 5 | 0.84 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD1 | 5 | 0.84 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD2 | 5 | 0.84 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD1 | 5 | 0.84 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD2 | 5 | 0.84 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HD2 | 15 | 0.84 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 15 | 0.83 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 15 | 0.83 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 3 | 0.83 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 3 | 0.83 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 13 | 0.83 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 13 | 0.83 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HE2 | 4 | 0.82 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 10 | 0.82 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 10 | 0.82 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 10 | 0.82 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 10 | 0.82 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 5 | 0.82 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 5 | 0.82 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 13 | 0.81 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 13 | 0.81 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 13 | 0.81 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 13 | 0.81 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 13 | 0.81 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 13 | 0.81 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 7 | 0.81 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 7 | 0.81 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 7 | 0.81 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 7 | 0.81 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 14 | 0.81 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 14 | 0.81 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 14 | 0.81 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 14 | 0.81 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 14 | 0.81 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 14 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 15 | 0.81 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 15 | 0.81 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 15 | 0.81 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 15 | 0.81 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 17 | 0.8 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 1 | 0.8 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 1 | 0.8 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 7 | 0.8 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 7 | 0.8 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 19 | 0.8 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 19 | 0.8 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 9 | 0.79 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 20 | 0.79 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 20 | 0.79 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 20 | 0.79 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 20 | 0.79 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 20 | 0.79 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 20 | 0.79 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 16 | 0.78 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 16 | 0.78 |
| (2,1) | 1:9:A:CYS:CB | 1:34:A:CYS:CB | 20 | 0.77 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 2 | 0.77 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 2 | 0.77 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 10 | 0.77 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 10 | 0.77 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 10 | 0.77 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 10 | 0.77 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 10 | 0.77 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 10 | 0.77 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 1 | 0.77 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 1 | 0.77 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 20 | 0.77 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 20 | 0.77 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 2 | 0.77 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 2 | 0.77 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 18 | 0.77 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 18 | 0.77 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HE1 | 6 | 0.77 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 12 | 0.76 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 9 | 0.76 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 9 | 0.76 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 9 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 9 | 0.76 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 20 | 0.75 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 20 | 0.75 |
| (1,421) | 1:49:A:VAL:HG13 | 2:121:B:TYS:HE1 | 8 | 0.75 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 17 | 0.75 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 17 | 0.75 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 17 | 0.75 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 17 | 0.75 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 17 | 0.75 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 17 | 0.75 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 9 | 0.75 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 9 | 0.75 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 8 | 0.75 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 8 | 0.75 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 8 | 0.75 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 8 | 0.75 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 8 | 0.74 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 8 | 0.74 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD1 | 19 | 0.74 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD2 | 19 | 0.74 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD1 | 14 | 0.74 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 4 | 0.74 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 4 | 0.74 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 14 | 0.74 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 14 | 0.74 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 14 | 0.74 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 14 | 0.74 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 14 | 0.74 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 14 | 0.74 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 2 | 0.73 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 2 | 0.73 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 4 | 0.73 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 4 | 0.73 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 5 | 0.73 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 5 | 0.73 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 5 | 0.73 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 5 | 0.73 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 14 | 0.73 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 14 | 0.73 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 14 | 0.73 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 14 | 0.73 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 10 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 17 | 0.72 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 17 | 0.72 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 17 | 0.72 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 7 | 0.72 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 7 | 0.72 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 12 | 0.72 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 12 | 0.72 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 14 | 0.72 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 14 | 0.72 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 15 | 0.72 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 15 | 0.72 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE1 | 4 | 0.72 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE2 | 4 | 0.72 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 12 | 0.71 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 12 | 0.71 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 13 | 0.71 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 13 | 0.71 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 15 | 0.71 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 15 | 0.71 |
| (1,1507) | 2:306:D:ILE:HD11 | 2:307:D:TYS:H | 5 | 0.71 |
| (1,1507) | 2:306:D:ILE:HD12 | 2:307:D:TYS:H | 5 | 0.71 |
| (1,1507) | 2:306:D:ILE:HD13 | 2:307:D:TYS:H | 5 | 0.71 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 11 | 0.71 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 11 | 0.71 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 18 | 0.71 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 18 | 0.71 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 18 | 0.71 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 18 | 0.71 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 13 | 0.71 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 13 | 0.71 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 13 | 0.71 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 13 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 6 | 0.71 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 6 | 0.71 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 19 | 0.71 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 19 | 0.71 |
| (1,754) | 2:107:B:TYS:HE2 | 1:223:C:VAL:HG22 | 4 | 0.71 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 9 | 0.71 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 17 | 0.71 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 17 | 0.71 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 2 | 0.71 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 2 | 0.71 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 8 | 0.71 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 8 | 0.71 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 8 | 0.71 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 8 | 0.71 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 8 | 0.71 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 8 | 0.71 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 5 | 0.71 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 5 | 0.71 |
| (1,23) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HD1 | 5 | 0.71 |
| (1,23) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HD2 | 5 | 0.71 |
| (1,23) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HD1 | 5 | 0.71 |
| (1,23) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HD2 | 5 | 0.71 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 4 | 0.7 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 7 | 0.7 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 12 | 0.7 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 13 | 0.7 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 6 | 0.7 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 6 | 0.7 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 8 | 0.7 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 8 | 0.7 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 20 | 0.7 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 20 | 0.7 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 20 | 0.7 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 20 | 0.7 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 4 | 0.7 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 4 | 0.7 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 4 | 0.7 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 4 | 0.7 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 20 | 0.7 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 20 | 0.7 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 3 | 0.7 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 3 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 8 | 0.7 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 8 | 0.7 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 18 | 0.7 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 18 | 0.7 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 18 | 0.7 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 18 | 0.7 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 18 | 0.7 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 18 | 0.7 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 17 | 0.7 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 17 | 0.7 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 17 | 0.7 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 17 | 0.7 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 6 | 0.7 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 6 | 0.7 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 6 | 0.7 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 6 | 0.7 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 1 | 0.69 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 4 | 0.69 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 18 | 0.69 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 11 | 0.69 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 11 | 0.69 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 14 | 0.69 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 14 | 0.69 |
| (1,1507) | 2:306:D:ILE:HD11 | 2:307:D:TYS:H | 13 | 0.69 |
| (1,1507) | 2:306:D:ILE:HD12 | 2:307:D:TYS:H | 13 | 0.69 |
| (1,1507) | 2:306:D:ILE:HD13 | 2:307:D:TYS:H | 13 | 0.69 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 9 | 0.69 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 9 | 0.69 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 5 | 0.69 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 5 | 0.69 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 9 | 0.69 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 9 | 0.69 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 16 | 0.69 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 16 | 0.69 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD1 | 17 | 0.69 |
| (1,139) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HD1 | 20 | 0.69 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 13 | 0.68 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 15 | 0.68 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 2 | 0.68 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 2 | 0.68 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 5 | 0.68 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 5 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 4 | 0.68 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 4 | 0.68 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HE2 | 12 | 0.68 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 18 | 0.68 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 18 | 0.68 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 2 | 0.68 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 2 | 0.68 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 10 | 0.68 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 10 | 0.68 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 13 | 0.68 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 13 | 0.68 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE1 | 3 | 0.68 |
| (1,16) | 1:10:A:PRO:HB3 | 2:112:B:TYS:HE2 | 3 | 0.68 |
| (2,13) | 1:209:C:CYS:CB | 1:234:C:CYS:CB | 19 | 0.67 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD1 | 5 | 0.67 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD2 | 5 | 0.67 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD1 | 5 | 0.67 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD2 | 5 | 0.67 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD1 | 5 | 0.67 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD2 | 5 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 4 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 4 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 4 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 4 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 4 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 4 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 17 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 17 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 17 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 17 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 17 | 0.67 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 17 | 0.67 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 16 | 0.67 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 16 | 0.67 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 14 | 0.67 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 14 | 0.67 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 14 | 0.67 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 2 | 0.67 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 2 | 0.67 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 2 | 0.67 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 2 | 0.67 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 13 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 13 | 0.66 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE2 | 6 | 0.66 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HD2 | 16 | 0.66 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 2 | 0.65 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 8 | 0.65 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 15 | 0.65 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 12 | 0.65 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 12 | 0.65 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 12 | 0.65 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 12 | 0.65 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 12 | 0.65 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 12 | 0.65 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 12 | 0.64 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 12 | 0.64 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD1 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD2 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD1 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD2 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD1 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD2 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD1 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD2 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD1 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD2 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD1 | 9 | 0.64 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD2 | 9 | 0.64 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 5 | 0.64 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 5 | 0.64 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 5 | 0.64 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 5 | 0.64 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 5 | 0.64 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 5 | 0.64 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 8 | 0.64 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 8 | 0.64 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 16 | 0.64 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 16 | 0.64 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 16 | 0.64 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 16 | 0.64 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 16 | 0.64 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 16 | 0.64 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 20 | 0.63 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 9 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 9 | 0.63 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 9 | 0.63 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 9 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 3 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 3 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 3 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 3 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 3 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 3 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 5 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 5 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 5 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 5 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 5 | 0.63 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 5 | 0.63 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD1 | 16 | 0.63 |
| (1,752) | 2:107:B:TYS:HA | 2:107:B:TYS:HD2 | 16 | 0.63 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 16 | 0.62 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 19 | 0.62 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 20 | 0.62 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 20 | 0.62 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE1 | 5 | 0.62 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE2 | 5 | 0.62 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE1 | 5 | 0.62 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE2 | 5 | 0.62 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE1 | 5 | 0.62 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE2 | 5 | 0.62 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 20 | 0.62 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 20 | 0.62 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 16 | 0.62 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 16 | 0.62 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 17 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 17 | 0.62 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 17 | 0.62 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 17 | 0.62 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 17 | 0.62 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 6 | 0.61 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 7 | 0.61 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 7 | 0.61 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 7 | 0.61 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 7 | 0.61 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 8 | 0.61 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 8 | 0.61 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 11 | 0.61 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 11 | 0.61 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 11 | 0.61 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 11 | 0.61 |
| (1,881) | 1:210:C:PRO:HA | 2:312:D:TYS:HD1 | 15 | 0.61 |
| (1,881) | 1:210:C:PRO:HA | 2:312:D:TYS:HD2 | 15 | 0.61 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 6 | 0.61 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 6 | 0.61 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 6 | 0.61 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 6 | 0.61 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 6 | 0.61 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 6 | 0.61 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 12 | 0.61 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 12 | 0.61 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 12 | 0.61 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 12 | 0.61 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 3 | 0.61 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 3 | 0.61 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 3 | 0.61 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 3 | 0.61 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 3 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 3 | 0.61 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 4 | 0.61 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 4 | 0.61 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 4 | 0.61 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 4 | 0.61 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 4 | 0.61 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 4 | 0.61 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 18 | 0.6 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 9 | 0.6 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 9 | 0.6 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 9 | 0.6 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 9 | 0.6 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 6 | 0.6 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 6 | 0.6 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 2 | 0.6 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 2 | 0.6 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 2 | 0.6 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 2 | 0.6 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE1 | 2 | 0.6 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE2 | 2 | 0.6 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 6 | 0.6 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD1 | 5 | 0.6 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD2 | 5 | 0.6 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD1 | 5 | 0.6 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD2 | 5 | 0.6 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD1 | 5 | 0.6 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD2 | 5 | 0.6 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 5 | 0.6 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 5 | 0.6 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 5 | 0.6 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 5 | 0.6 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 5 | 0.6 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 5 | 0.6 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 16 | 0.59 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 2 | 0.59 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 2 | 0.59 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE1 | 19 | 0.59 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE2 | 19 | 0.59 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE1 | 19 | 0.59 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE2 | 19 | 0.59 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE1 | 19 | 0.59 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE2 | 19 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1507) | 2:306:D:ILE:HD11 | 2:307:D:TYS:H | 15 | 0.59 |
| (1,1507) | 2:306:D:ILE:HD12 | 2:307:D:TYS:H | 15 | 0.59 |
| (1,1507) | 2:306:D:ILE:HD13 | 2:307:D:TYS:H | 15 | 0.59 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 17 | 0.59 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 17 | 0.59 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 14 | 0.59 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 14 | 0.59 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 14 | 0.59 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 14 | 0.59 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 14 | 0.59 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 14 | 0.59 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 7 | 0.59 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 7 | 0.59 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 7 | 0.59 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 7 | 0.59 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 7 | 0.59 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 7 | 0.59 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD2 | 10 | 0.59 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE2 | 12 | 0.59 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 9 | 0.58 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 18 | 0.58 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 18 | 0.58 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 3 | 0.58 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 3 | 0.58 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE1 | 20 | 0.58 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE2 | 20 | 0.58 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE1 | 20 | 0.58 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE2 | 20 | 0.58 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE1 | 20 | 0.58 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE2 | 20 | 0.58 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 1 | 0.58 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 1 | 0.58 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 16 | 0.58 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 16 | 0.58 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 16 | 0.58 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 16 | 0.58 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 16 | 0.58 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 16 | 0.58 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 7 | 0.58 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 7 | 0.58 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 7 | 0.58 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 7 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 14 | 0.58 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 14 | 0.58 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 14 | 0.58 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 14 | 0.58 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 7 | 0.58 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 7 | 0.58 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 7 | 0.58 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 7 | 0.58 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 7 | 0.58 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 7 | 0.58 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 2 | 0.57 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 5 | 0.57 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 5 | 0.57 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 5 | 0.57 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 5 | 0.57 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 7 | 0.57 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 7 | 0.57 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 18 | 0.57 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 18 | 0.57 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 11 | 0.57 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 11 | 0.57 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 11 | 0.57 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 11 | 0.57 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 11 | 0.57 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 11 | 0.57 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 11 | 0.57 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 11 | 0.57 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 9 | 0.56 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 16 | 0.56 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 16 | 0.56 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 16 | 0.56 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 16 | 0.56 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HE2 | 9 | 0.56 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE1 | 7 | 0.56 |
| (1,787) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HE2 | 7 | 0.56 |
| (1,754) | 2:107:B:TYS:HD1 | 1:223:C:VAL:HG22 | 12 | 0.56 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 4 | 0.56 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 4 | 0.56 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 4 | 0.56 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 4 | 0.56 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 4 | 0.56 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 4 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 18 | 0.56 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 18 | 0.56 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 18 | 0.56 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 18 | 0.56 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 18 | 0.56 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 18 | 0.56 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 20 | 0.56 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 20 | 0.56 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 20 | 0.56 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 20 | 0.56 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 20 | 0.56 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 20 | 0.56 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 6 | 0.55 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 18 | 0.55 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 18 | 0.55 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD1 | 19 | 0.55 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD2 | 19 | 0.55 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD1 | 19 | 0.55 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD2 | 19 | 0.55 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD1 | 19 | 0.55 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD2 | 19 | 0.55 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 7 | 0.55 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 7 | 0.55 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 13 | 0.55 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 13 | 0.55 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 13 | 0.55 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 13 | 0.55 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 10 | 0.55 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 10 | 0.55 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 10 | 0.55 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 10 | 0.55 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 6 | 0.55 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 6 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 6 | 0.55 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 14 | 0.55 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 14 | 0.55 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE1 | 1 | 0.55 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 6 | 0.55 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 6 | 0.55 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 7 | 0.54 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 6 | 0.54 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 6 | 0.54 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 8 | 0.54 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 8 | 0.54 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 16 | 0.54 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 16 | 0.54 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 16 | 0.54 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 16 | 0.54 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 16 | 0.54 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 16 | 0.54 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 12 | 0.54 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 12 | 0.54 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 12 | 0.54 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 12 | 0.54 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 18 | 0.54 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 18 | 0.54 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 18 | 0.54 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 18 | 0.54 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 2 | 0.54 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 2 | 0.54 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 2 | 0.54 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 2 | 0.54 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 2 | 0.54 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 2 | 0.54 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 18 | 0.54 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 18 | 0.54 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 18 | 0.54 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 18 | 0.54 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 7 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 7 | 0.54 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 7 | 0.54 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 11 | 0.53 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 19 | 0.53 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 3 | 0.53 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 3 | 0.53 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 13 | 0.53 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 13 | 0.53 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 19 | 0.53 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 19 | 0.53 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 3 | 0.53 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 3 | 0.53 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 20 | 0.53 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 20 | 0.53 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 20 | 0.53 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 20 | 0.53 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 4 | 0.53 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 4 | 0.53 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 11 | 0.53 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 11 | 0.53 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 8 | 0.53 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 8 | 0.53 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 9 | 0.52 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 9 | 0.52 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 19 | 0.52 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 19 | 0.52 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 5 | 0.52 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 5 | 0.52 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 5 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 5 | 0.52 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 5 | 0.52 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 5 | 0.52 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 13 | 0.52 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 13 | 0.52 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 11 | 0.52 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 11 | 0.52 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 20 | 0.52 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 20 | 0.52 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 20 | 0.52 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 20 | 0.52 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 20 | 0.52 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 20 | 0.52 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE1 | 19 | 0.52 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE2 | 19 | 0.52 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE1 | 19 | 0.52 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE2 | 19 | 0.52 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE1 | 19 | 0.52 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE2 | 19 | 0.52 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 16 | 0.52 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 16 | 0.52 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 16 | 0.52 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 16 | 0.52 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 15 | 0.52 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 15 | 0.52 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 9 | 0.52 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 9 | 0.52 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 9 | 0.52 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 9 | 0.52 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 11 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE1 | 4 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE2 | 4 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE1 | 4 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE2 | 4 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE1 | 4 | 0.51 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE2 | 4 | 0.51 |
| (1,1507) | 2:306:D:ILE:HD11 | 2:307:D:TYS:H | 14 | 0.51 |
| (1,1507) | 2:306:D:ILE:HD12 | 2:307:D:TYS:H | 14 | 0.51 |
| (1,1507) | 2:306:D:ILE:HD13 | 2:307:D:TYS:H | 14 | 0.51 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 6 | 0.51 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 6 | 0.51 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 6 | 0.51 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 6 | 0.51 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 6 | 0.51 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 6 | 0.51 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 9 | 0.51 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 9 | 0.51 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 7 | 0.51 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 7 | 0.51 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 17 | 0.51 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 17 | 0.51 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 6 | 0.51 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 6 | 0.51 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 13 | 0.51 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 13 | 0.51 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 13 | 0.51 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 13 | 0.51 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 13 | 0.51 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 13 | 0.51 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 7 | 0.5 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 7 | 0.5 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 1 | 0.5 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 1 | 0.5 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 9 | 0.5 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 9 | 0.5 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 10 | 0.5 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 10 | 0.5 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 16 | 0.5 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 16 | 0.5 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 16 | 0.5 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 16 | 0.5 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 16 | 0.5 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 16 | 0.5 |
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD1 | 3 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,954) | 1:218:C:VAL:HB | 2:321:D:TYS:HD2 | 3 | 0.5 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 13 | 0.5 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 13 | 0.5 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 13 | 0.5 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 13 | 0.5 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE1 | 9 | 0.5 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE2 | 9 | 0.5 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 18 | 0.5 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 18 | 0.5 |
| (2,16) | 1:211:C:CYS:CB | 1:250:C:CYS:CB | 14 | 0.49 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 10 | 0.49 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 14 | 0.49 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 14 | 0.49 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 14 | 0.49 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 14 | 0.49 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 16 | 0.49 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 16 | 0.49 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD2 | 13 | 0.49 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 15 | 0.49 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 15 | 0.49 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 15 | 0.49 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 15 | 0.49 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 3 | 0.49 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 3 | 0.49 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 3 | 0.49 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 3 | 0.49 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 3 | 0.49 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 3 | 0.49 |
| (1,139) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HD2 | 18 | 0.49 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 15 | 0.48 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 15 | 0.48 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 15 | 0.48 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 15 | 0.48 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 15 | 0.48 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 15 | 0.48 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 12 | 0.48 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 12 | 0.48 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 12 | 0.48 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 12 | 0.48 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD1 | 17 | 0.48 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD2 | 17 | 0.48 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD1 | 17 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD2 | 17 | 0.48 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD1 | 17 | 0.48 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD2 | 17 | 0.48 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 7 | 0.48 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 7 | 0.48 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 10 | 0.47 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 10 | 0.47 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 10 | 0.47 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 10 | 0.47 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 7 | 0.47 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 7 | 0.47 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 2 | 0.47 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 2 | 0.47 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 2 | 0.47 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 2 | 0.47 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 3 | 0.47 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 3 | 0.47 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 3 | 0.47 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 3 | 0.47 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 4 | 0.47 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 4 | 0.47 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 4 | 0.47 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 4 | 0.47 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 7 | 0.47 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 7 | 0.47 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 7 | 0.47 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 7 | 0.47 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 2 | 0.47 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 2 | 0.47 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 4 | 0.47 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 4 | 0.47 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 13 | 0.47 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 13 | 0.47 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 13 | 0.47 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE1 | 17 | 0.47 |
| (1,425) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HE2 | 17 | 0.47 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE1 | 17 | 0.47 |
| (1,425) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HE2 | 17 | 0.47 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE1 | 17 | 0.47 |
| (1,425) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HE2 | 17 | 0.47 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 10 | 0.47 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 10 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 10 | 0.47 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 10 | 0.47 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 10 | 0.47 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 10 | 0.47 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 2 | 0.47 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 2 | 0.47 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 2 | 0.47 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 2 | 0.47 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 8 | 0.46 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 8 | 0.46 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 8 | 0.46 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 8 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 10 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 10 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 10 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 10 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 10 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 10 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 14 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 14 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 14 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 14 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 14 | 0.46 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 14 | 0.46 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 1 | 0.46 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 1 | 0.46 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 1 | 0.46 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 1 | 0.46 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 1 | 0.46 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 1 | 0.46 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 11 | 0.46 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 11 | 0.46 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 16 | 0.46 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 16 | 0.46 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 16 | 0.46 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 16 | 0.46 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 3 | 0.46 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 3 | 0.46 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 18 | 0.46 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 18 | 0.46 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 18 | 0.46 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 18 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 1 | 0.46 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 1 | 0.46 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 6 | 0.46 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 6 | 0.46 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 6 | 0.46 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 6 | 0.46 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 6 | 0.46 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 6 | 0.46 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 15 | 0.46 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 15 | 0.46 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 15 | 0.46 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 15 | 0.46 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 11 | 0.45 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 11 | 0.45 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 11 | 0.45 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 11 | 0.45 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 11 | 0.45 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 11 | 0.45 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 15 | 0.45 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 15 | 0.45 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 15 | 0.45 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 15 | 0.45 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 15 | 0.45 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 15 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 12 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 12 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 12 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 12 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 12 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 12 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 15 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 15 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 15 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 15 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 15 | 0.45 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 15 | 0.45 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 12 | 0.45 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 12 | 0.45 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 12 | 0.45 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 12 | 0.45 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 7 | 0.45 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 7 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 7 | 0.45 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 7 | 0.45 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 9 | 0.44 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 9 | 0.44 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 11 | 0.44 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 11 | 0.44 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 11 | 0.44 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 11 | 0.44 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 13 | 0.44 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 13 | 0.44 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 11 | 0.44 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 11 | 0.44 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 11 | 0.44 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 11 | 0.44 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 16 | 0.43 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 16 | 0.43 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 14 | 0.43 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 14 | 0.43 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 14 | 0.43 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 14 | 0.43 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 14 | 0.43 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 14 | 0.43 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 7 | 0.43 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 7 | 0.43 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 7 | 0.43 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 7 | 0.43 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 7 | 0.43 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 7 | 0.43 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 19 | 0.43 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 19 | 0.43 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 19 | 0.43 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 19 | 0.43 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 19 | 0.43 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 19 | 0.43 |
| (1,881) | 1:210:C:PRO:HA | 2:312:D:TYS:HD1 | 7 | 0.43 |
| (1,881) | 1:210:C:PRO:HA | 2:312:D:TYS:HD2 | 7 | 0.43 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 15 | 0.43 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 15 | 0.43 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 10 | 0.43 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 10 | 0.43 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 10 | 0.43 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 10 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 10 | 0.43 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 10 | 0.43 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 2 | 0.43 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 2 | 0.43 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 2 | 0.43 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 2 | 0.43 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 2 | 0.43 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 2 | 0.43 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 17 | 0.43 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 17 | 0.43 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 17 | 0.43 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 17 | 0.43 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 17 | 0.43 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 17 | 0.43 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 8 | 0.43 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 8 | 0.43 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 8 | 0.43 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 8 | 0.43 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 8 | 0.43 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 8 | 0.43 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 7 | 0.42 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 5 | 0.42 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 17 | 0.42 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 17 | 0.42 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 17 | 0.42 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 17 | 0.42 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 1 | 0.42 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 1 | 0.42 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 11 | 0.42 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 11 | 0.42 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 11 | 0.42 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 11 | 0.42 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 11 | 0.42 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 11 | 0.42 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 6 | 0.42 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 6 | 0.42 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 20 | 0.42 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 20 | 0.42 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 20 | 0.42 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 20 | 0.42 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 20 | 0.42 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 20 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 2 | 0.42 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 2 | 0.42 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 11 | 0.41 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 13 | 0.41 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 6 | 0.41 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 6 | 0.41 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 6 | 0.41 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 6 | 0.41 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 12 | 0.41 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 12 | 0.41 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 12 | 0.41 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 12 | 0.41 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 1 | 0.41 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 1 | 0.41 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE1 | 10 | 0.41 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE2 | 10 | 0.41 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE1 | 10 | 0.41 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE2 | 10 | 0.41 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE1 | 10 | 0.41 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE2 | 10 | 0.41 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE1 | 10 | 0.41 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE2 | 10 | 0.41 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE1 | 10 | 0.41 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE2 | 10 | 0.41 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 13 | 0.41 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 2 | 0.41 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 2 | 0.41 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 5 | 0.41 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 5 | 0.41 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 5 | 0.41 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 5 | 0.41 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 5 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 5 | 0.41 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE1 | 5 | 0.41 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 1 | 0.41 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 1 | 0.41 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 12 | 0.41 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 12 | 0.41 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 16 | 0.4 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 13 | 0.4 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 19 | 0.4 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 13 | 0.4 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 1 | 0.4 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 1 | 0.4 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 5 | 0.4 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 5 | 0.4 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 17 | 0.4 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 17 | 0.4 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 4 | 0.4 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 4 | 0.4 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 20 | 0.4 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 20 | 0.4 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 20 | 0.4 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 20 | 0.4 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 9 | 0.4 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 9 | 0.4 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 7 | 0.39 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 11 | 0.39 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 15 | 0.39 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 15 | 0.39 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 15 | 0.39 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 15 | 0.39 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 11 | 0.39 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 11 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 15 | 0.39 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 15 | 0.39 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 15 | 0.39 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 15 | 0.39 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 15 | 0.39 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 15 | 0.39 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD1 | 11 | 0.39 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 17 | 0.39 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 17 | 0.39 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 8 | 0.39 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 8 | 0.39 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 14 | 0.39 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 14 | 0.39 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD1 | 19 | 0.39 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD2 | 19 | 0.39 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD1 | 19 | 0.39 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD2 | 19 | 0.39 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD1 | 19 | 0.39 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD2 | 19 | 0.39 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 11 | 0.39 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 11 | 0.39 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 11 | 0.39 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 11 | 0.39 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 11 | 0.39 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 11 | 0.39 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 17 | 0.39 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 17 | 0.39 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 17 | 0.39 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 17 | 0.39 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 17 | 0.39 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 17 | 0.39 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD1 | 12 | 0.39 |
| (1,287) | 1:29:A:LEU:HB2 | 2:112:B:TYS:HD2 | 12 | 0.39 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD1 | 12 | 0.39 |
| (1,287) | 1:29:A:LEU:HB3 | 2:112:B:TYS:HD2 | 12 | 0.39 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 14 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 14 | 0.39 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 14 | 0.39 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE1 | 4 | 0.39 |
| (1,24) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HE2 | 4 | 0.39 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE1 | 4 | 0.39 |
| (1,24) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HE2 | 4 | 0.39 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 7 | 0.38 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 16 | 0.38 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 19 | 0.38 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 20 | 0.38 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 7 | 0.38 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 12 | 0.38 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 16 | 0.38 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 5 | 0.38 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 19 | 0.38 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 19 | 0.38 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 16 | 0.38 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 16 | 0.38 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 12 | 0.38 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 12 | 0.38 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 13 | 0.38 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 13 | 0.38 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 13 | 0.38 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 13 | 0.38 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 13 | 0.38 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 13 | 0.38 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 5 | 0.38 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 5 | 0.38 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 5 | 0.38 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 5 | 0.38 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 16 | 0.38 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 16 | 0.38 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 16 | 0.38 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 16 | 0.38 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 19 | 0.38 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 19 | 0.38 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 19 | 0.38 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 19 | 0.38 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 7 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 7 | 0.38 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 4 | 0.38 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE1 | 14 | 0.38 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 18 | 0.38 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 18 | 0.38 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 18 | 0.38 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 18 | 0.38 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 16 | 0.38 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 16 | 0.38 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD1 | 6 | 0.38 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD2 | 6 | 0.38 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 13 | 0.37 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 13 | 0.37 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 12 | 0.37 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 10 | 0.37 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 16 | 0.37 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 7 | 0.37 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 11 | 0.37 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 4 | 0.37 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 6 | 0.37 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 13 | 0.37 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 12 | 0.37 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 6 | 0.37 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 4 | 0.37 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 4 | 0.37 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 4 | 0.37 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 4 | 0.37 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE1 | 7 | 0.37 |
| (1,1115) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HE2 | 7 | 0.37 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE1 | 7 | 0.37 |
| (1,1115) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HE2 | 7 | 0.37 |
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE1 | 7 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1115) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HE2 | 7 | 0.37 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 1 | 0.37 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 1 | 0.37 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 9 | 0.37 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 9 | 0.37 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 1 | 0.37 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 1 | 0.37 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 1 | 0.37 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 1 | 0.37 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 1 | 0.37 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 1 | 0.37 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 3 | 0.37 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 3 | 0.37 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE1 | 7 | 0.37 |
| (1,81) | 1:18:A:VAL:HB | 2:121:B:TYS:HE2 | 7 | 0.37 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 5 | 0.36 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 5 | 0.36 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 20 | 0.36 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 19 | 0.36 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 6 | 0.36 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 18 | 0.36 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 14 | 0.36 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 11 | 0.36 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 12 | 0.36 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 12 | 0.36 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 16 | 0.36 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 7 | 0.36 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 8 | 0.36 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 5 | 0.36 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 12 | 0.36 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 20 | 0.36 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 20 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 20 | 0.36 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 20 | 0.36 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD1 | 17 | 0.36 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD2 | 17 | 0.36 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD1 | 17 | 0.36 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD2 | 17 | 0.36 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD1 | 17 | 0.36 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD2 | 17 | 0.36 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 12 | 0.36 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 12 | 0.36 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 12 | 0.36 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 12 | 0.36 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 12 | 0.36 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 12 | 0.36 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD1 | 4 | 0.36 |
| (1,1108) | 1:229:C:LEU:HB2 | 2:312:D:TYS:HD2 | 4 | 0.36 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD1 | 4 | 0.36 |
| (1,1108) | 1:229:C:LEU:HB3 | 2:312:D:TYS:HD2 | 4 | 0.36 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD1 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD2 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD1 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD2 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD1 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD2 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD1 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD2 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD1 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD2 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD1 | 20 | 0.36 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD2 | 20 | 0.36 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 4 | 0.36 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 4 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 11 | 0.35 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 2 | 0.35 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 4 | 0.35 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 6 | 0.35 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 10 | 0.35 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 15 | 0.35 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 14 | 0.35 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 20 | 0.35 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 1 | 0.35 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 13 | 0.35 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 13 | 0.35 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 19 | 0.35 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 2 | 0.35 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 16 | 0.35 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 20 | 0.35 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 11 | 0.35 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 3 | 0.35 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 3 | 0.35 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 3 | 0.35 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 3 | 0.35 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 5 | 0.35 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 5 | 0.35 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 13 | 0.35 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 13 | 0.35 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 11 | 0.35 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 11 | 0.35 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 14 | 0.35 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 14 | 0.35 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 19 | 0.35 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 19 | 0.35 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 7 | 0.35 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 7 | 0.35 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 7 | 0.35 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 7 | 0.35 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 7 | 0.35 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 7 | 0.35 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 6 | 0.35 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 6 | 0.35 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 6 | 0.35 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 6 | 0.35 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 10 | 0.35 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 10 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 3 | 0.35 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 3 | 0.35 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 15 | 0.35 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 15 | 0.35 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 15 | 0.35 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 15 | 0.35 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 15 | 0.35 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 15 | 0.35 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 12 | 0.35 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 12 | 0.35 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 1 | 0.34 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 4 | 0.34 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 5 | 0.34 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 13 | 0.34 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 16 | 0.34 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 20 | 0.34 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 11 | 0.34 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 14 | 0.34 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 18 | 0.34 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 9 | 0.34 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 19 | 0.34 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 7 | 0.34 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 6 | 0.34 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 13 | 0.34 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 18 | 0.34 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 4 | 0.34 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 4 | 0.34 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 10 | 0.34 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 10 | 0.34 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HE1 | 20 | 0.34 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE1 | 17 | 0.34 |
| (1,1087) | 1:227:C:LYS:HE2 | 2:312:D:TYS:HE2 | 17 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE1 | 17 | 0.34 |
| (1,1087) | 1:227:C:LYS:HE3 | 2:312:D:TYS:HE2 | 17 | 0.34 |
| (1,896) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HD1 | 15 | 0.34 |
| (1,896) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HD2 | 15 | 0.34 |
| (1,896) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HD1 | 15 | 0.34 |
| (1,896) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HD2 | 15 | 0.34 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 20 | 0.34 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 20 | 0.34 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 20 | 0.34 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 20 | 0.34 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE1 | 10 | 0.34 |
| (1,237) | 1:27:A:LYS:HG2 | 2:112:B:TYS:HE2 | 10 | 0.34 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 5 | 0.33 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 11 | 0.33 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 15 | 0.33 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 6 | 0.33 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 16 | 0.33 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 20 | 0.33 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 6 | 0.33 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 2 | 0.33 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 5 | 0.33 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 14 | 0.33 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 2 | 0.33 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 3 | 0.33 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 9 | 0.33 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 13 | 0.33 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 9 | 0.33 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 20 | 0.33 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 17 | 0.33 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 4 | 0.33 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 14 | 0.33 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD11 | 14 | 0.33 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD12 | 14 | 0.33 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD13 | 14 | 0.33 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 4 | 0.33 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 4 | 0.33 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 4 | 0.33 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 4 | 0.33 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 4 | 0.33 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 4 | 0.33 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 14 | 0.33 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 14 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 14 | 0.33 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 14 | 0.33 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 11 | 0.33 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 11 | 0.33 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 20 | 0.33 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 20 | 0.33 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 16 | 0.33 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 9 | 0.33 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 9 | 0.33 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 9 | 0.33 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 9 | 0.33 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 9 | 0.33 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 9 | 0.33 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 16 | 0.33 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 16 | 0.33 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 16 | 0.33 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 16 | 0.33 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 16 | 0.33 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 16 | 0.33 |
| (1,421) | 1:49:A:VAL:HG13 | 2:121:B:TYS:HE1 | 12 | 0.33 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 11 | 0.32 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 8 | 0.32 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 17 | 0.32 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 2 | 0.32 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 5 | 0.32 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 6 | 0.32 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 14 | 0.32 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 17 | 0.32 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 4 | 0.32 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 7 | 0.32 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 6 | 0.32 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 16 | 0.32 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 12 | 0.32 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 17 | 0.32 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 19 | 0.32 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 6 | 0.32 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 8 | 0.32 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 7 | 0.32 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 12 | 0.32 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 19 | 0.32 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 20 | 0.32 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 19 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 12 | 0.32 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 12 | 0.32 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 10 | 0.32 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 7 | 0.32 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 7 | 0.32 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 7 | 0.32 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 7 | 0.32 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 18 | 0.32 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 18 | 0.32 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 18 | 0.32 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 18 | 0.32 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE1 | 20 | 0.32 |
| (1,1555) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HE2 | 20 | 0.32 |
| (1,1514) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HD1 | 5 | 0.32 |
| (1,1514) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HD2 | 5 | 0.32 |
| (1,1514) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HD1 | 5 | 0.32 |
| (1,1514) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HD2 | 5 | 0.32 |
| (1,1514) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HD1 | 5 | 0.32 |
| (1,1514) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HD2 | 5 | 0.32 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 3 | 0.32 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 3 | 0.32 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 12 | 0.32 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 12 | 0.32 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 16 | 0.32 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 16 | 0.32 |
| (1,1502) | 2:306:D:ILE:HA | 2:307:D:TYS:H | 13 | 0.32 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE1 | 2 | 0.32 |
| (1,890) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HE2 | 2 | 0.32 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 10 | 0.32 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 10 | 0.32 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 10 | 0.32 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 10 | 0.32 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 11 | 0.32 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 11 | 0.32 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 2 | 0.32 |
| (1,734) | 2:106:B:ILE:HA | 2:106:B:ILE:HD11 | 14 | 0.32 |
| (1,734) | 2:106:B:ILE:HA | 2:106:B:ILE:HD12 | 14 | 0.32 |
| (1,734) | 2:106:B:ILE:HA | 2:106:B:ILE:HD13 | 14 | 0.32 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 4 | 0.32 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 4 | 0.32 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 4 | 0.32 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 4 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 4 | 0.32 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 4 | 0.32 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 17 | 0.31 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 13 | 0.31 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 1 | 0.31 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 2 | 0.31 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 7 | 0.31 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 11 | 0.31 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 16 | 0.31 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 16 | 0.31 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 2 | 0.31 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 18 | 0.31 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 11 | 0.31 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 13 | 0.31 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 15 | 0.31 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 16 | 0.31 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 20 | 0.31 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 17 | 0.31 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 2 | 0.31 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 4 | 0.31 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 5 | 0.31 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 8 | 0.31 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 10 | 0.31 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 9 | 0.31 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 17 | 0.31 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 14 | 0.31 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 19 | 0.31 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 2 | 0.31 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 3 | 0.31 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 1 | 0.31 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 19 | 0.31 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 19 | 0.31 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 19 | 0.31 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 19 | 0.31 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 2 | 0.31 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 2 | 0.31 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 4 | 0.31 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 4 | 0.31 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 10 | 0.31 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 10 | 0.31 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 18 | 0.31 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 18 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 18 | 0.31 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 18 | 0.31 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 18 | 0.31 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 18 | 0.31 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 8 | 0.31 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 8 | 0.31 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 8 | 0.31 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 8 | 0.31 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 4 | 0.31 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 4 | 0.31 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 3 | 0.31 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 3 | 0.31 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 3 | 0.31 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 3 | 0.31 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 1 | 0.3 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 6 | 0.3 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 12 | 0.3 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 14 | 0.3 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 16 | 0.3 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 3 | 0.3 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 14 | 0.3 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 18 | 0.3 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 19 | 0.3 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 10 | 0.3 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 17 | 0.3 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 8 | 0.3 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 14 | 0.3 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 17 | 0.3 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 20 | 0.3 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 14 | 0.3 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 13 | 0.3 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 5 | 0.3 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 11 | 0.3 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 12 | 0.3 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 17 | 0.3 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 4 | 0.3 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 1 | 0.3 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 2 | 0.3 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 3 | 0.3 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 9 | 0.3 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 12 | 0.3 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 13 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 14 | 0.3 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 20 | 0.3 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 6 | 0.3 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 9 | 0.3 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 14 | 0.3 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 18 | 0.3 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 13 | 0.3 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 20 | 0.3 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 3 | 0.3 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 4 | 0.3 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 9 | 0.3 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 17 | 0.3 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 6 | 0.3 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 5 | 0.3 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 17 | 0.3 |
| (1,1558) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 3 | 0.3 |
| (1,1558) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 3 | 0.3 |
| (1,1558) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HD1 | 3 | 0.3 |
| (1,1558) | 2:320:D:ASP:HB3 | 2:321:D:TYS:HD2 | 3 | 0.3 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE1 | 5 | 0.3 |
| (1,1551) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HE2 | 5 | 0.3 |
| (1,1516) | 2:307:D:TYS:H | 2:307:D:TYS:HB3 | 13 | 0.3 |
| (1,1516) | 2:307:D:TYS:H | 2:307:D:TYS:HB3 | 13 | 0.3 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 10 | 0.3 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 10 | 0.3 |
| (1,1504) | 2:306:D:ILE:HB | 2:307:D:TYS:H | 2 | 0.3 |
| (1,1504) | 2:306:D:ILE:HB | 2:307:D:TYS:H | 3 | 0.3 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 6 | 0.3 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 6 | 0.3 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 18 | 0.3 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 18 | 0.3 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 18 | 0.3 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 18 | 0.3 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 18 | 0.3 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 18 | 0.3 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE1 | 4 | 0.3 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE2 | 4 | 0.3 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE1 | 4 | 0.3 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE2 | 4 | 0.3 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE1 | 4 | 0.3 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE2 | 4 | 0.3 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 6 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 8 | 0.3 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 8 | 0.3 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 8 | 0.3 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 8 | 0.3 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 17 | 0.29 |
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 11 | 0.29 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 14 | 0.29 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 17 | 0.29 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 4 | 0.29 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 9 | 0.29 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 11 | 0.29 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 2 | 0.29 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 9 | 0.29 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 11 | 0.29 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 15 | 0.29 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 3 | 0.29 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 13 | 0.29 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 15 | 0.29 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 16 | 0.29 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 8 | 0.29 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 1 | 0.29 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 3 | 0.29 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 6 | 0.29 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 17 | 0.29 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 15 | 0.29 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 20 | 0.29 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 3 | 0.29 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 9 | 0.29 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 2 | 0.29 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 8 | 0.29 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 3 | 0.29 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 11 | 0.29 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 11 | 0.29 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 14 | 0.29 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 14 | 0.29 |
| (1,889) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HD1 | 19 | 0.29 |
| (1,889) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HD2 | 19 | 0.29 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HD2 | 2 | 0.29 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 9 | 0.29 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 9 | 0.29 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 9 | 0.29 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 9 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 12 | 0.29 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 12 | 0.29 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD1 | 15 | 0.29 |
| (1,742) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HD2 | 15 | 0.29 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD1 | 15 | 0.29 |
| (1,742) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HD2 | 15 | 0.29 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD1 | 15 | 0.29 |
| (1,742) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HD2 | 15 | 0.29 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 12 | 0.29 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 12 | 0.29 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 3 | 0.29 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE1 | 11 | 0.29 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 1 | 0.29 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 1 | 0.29 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 1 | 0.29 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 1 | 0.29 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 1 | 0.29 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 1 | 0.29 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 15 | 0.28 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 1 | 0.28 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 6 | 0.28 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 12 | 0.28 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 16 | 0.28 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 9 | 0.28 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 12 | 0.28 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 20 | 0.28 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 8 | 0.28 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 18 | 0.28 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 19 | 0.28 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 15 | 0.28 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 1 | 0.28 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 5 | 0.28 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 9 | 0.28 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 1 | 0.28 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 9 | 0.28 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 17 | 0.28 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 8 | 0.28 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 9 | 0.28 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 15 | 0.28 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 9 | 0.28 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 5 | 0.28 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 8 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 18 | 0.28 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 3 | 0.28 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 15 | 0.28 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 17 | 0.28 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 6 | 0.28 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 14 | 0.28 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 18 | 0.28 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 8 | 0.28 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 8 | 0.28 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 16 | 0.28 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 16 | 0.28 |
| (1,1502) | 2:306:D:ILE:HA | 2:307:D:TYS:H | 19 | 0.28 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 17 | 0.28 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 17 | 0.28 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 12 | 0.28 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE1 | 8 | 0.28 |
| (1,1229) | 1:247:C:ARG:HD2 | 2:321:D:TYS:HE2 | 8 | 0.28 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE1 | 8 | 0.28 |
| (1,1229) | 1:247:C:ARG:HD3 | 2:321:D:TYS:HE2 | 8 | 0.28 |
| (1,843) | 2:130:B:ARG:H | 2:130:B:ARG:HG2 | 15 | 0.28 |
| (1,843) | 2:130:B:ARG:H | 2:130:B:ARG:HG3 | 15 | 0.28 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE1 | 10 | 0.28 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE2 | 10 | 0.28 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE1 | 10 | 0.28 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE2 | 10 | 0.28 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE1 | 10 | 0.28 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE2 | 10 | 0.28 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 9 | 0.28 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD2 | 4 | 0.28 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD3 | 4 | 0.28 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD1 | 19 | 0.28 |
| (1,80) | 1:18:A:VAL:HB | 2:121:B:TYS:HD2 | 19 | 0.28 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 13 | 0.27 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 3 | 0.27 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 3 | 0.27 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 7 | 0.27 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 8 | 0.27 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 13 | 0.27 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 12 | 0.27 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 19 | 0.27 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 5 | 0.27 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 10 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 19 | 0.27 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 6 | 0.27 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 17 | 0.27 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 2 | 0.27 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 13 | 0.27 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 14 | 0.27 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 1 | 0.27 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 12 | 0.27 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 17 | 0.27 |
| (1,1504) | 2:306:D:ILE:HB | 2:307:D:TYS:H | 11 | 0.27 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 2 | 0.27 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 2 | 0.27 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 2 | 0.27 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 2 | 0.27 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 2 | 0.27 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 2 | 0.27 |
| (1,889) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HD1 | 7 | 0.27 |
| (1,889) | 1:210:C:PRO:HB3 | 2:312:D:TYS:HD2 | 7 | 0.27 |
| (1,809) | 2:125:B:LYS:H | 2:125:B:LYS:HG2 | 6 | 0.27 |
| (1,809) | 2:125:B:LYS:H | 2:125:B:LYS:HG3 | 6 | 0.27 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 16 | 0.27 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 16 | 0.27 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 8 | 0.27 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 8 | 0.27 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD2 | 6 | 0.27 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD3 | 6 | 0.27 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD2 | 8 | 0.27 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD3 | 8 | 0.27 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 15 | 0.27 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 15 | 0.27 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 15 | 0.27 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 15 | 0.27 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 15 | 0.27 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 15 | 0.27 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG21 | 20 | 0.27 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG22 | 20 | 0.27 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG23 | 20 | 0.27 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 6 | 0.27 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 6 | 0.27 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 6 | 0.27 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 6 | 0.27 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 6 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 6 | 0.27 |
| (1,113) | 1:20:A:ARG:HD2 | 1:23:A:VAL:H | 5 | 0.27 |
| (1,113) | 1:20:A:ARG:HD3 | 1:23:A:VAL:H | 5 | 0.27 |
| (1,23) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HD1 | 8 | 0.27 |
| (1,23) | 1:10:A:PRO:HG2 | 2:112:B:TYS:HD2 | 8 | 0.27 |
| (1,23) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HD1 | 8 | 0.27 |
| (1,23) | 1:10:A:PRO:HG3 | 2:112:B:TYS:HD2 | 8 | 0.27 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 20 | 0.26 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 15 | 0.26 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 12 | 0.26 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 6 | 0.26 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 15 | 0.26 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 4 | 0.26 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 3 | 0.26 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 6 | 0.26 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 6 | 0.26 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 14 | 0.26 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 2 | 0.26 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 7 | 0.26 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 13 | 0.26 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 20 | 0.26 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 3 | 0.26 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 18 | 0.26 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 7 | 0.26 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 15 | 0.26 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 16 | 0.26 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 3 | 0.26 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 9 | 0.26 |
| (2,4) | 1:11:A:CYS:CB | 1:50:A:CYS:CB | 14 | 0.26 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 10 | 0.26 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 10 | 0.26 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 8 | 0.26 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 8 | 0.26 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 6 | 0.26 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 6 | 0.26 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 13 | 0.26 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 13 | 0.26 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 13 | 0.26 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 13 | 0.26 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 13 | 0.26 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 13 | 0.26 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 5 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 5 | 0.26 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 16 | 0.26 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 16 | 0.26 |
| (1,588) | 1:60:A:GLU:HB3 | 1:60:A:GLU:HG3 | 1 | 0.26 |
| (1,159) | 1:24:A:LYS:HB2 | 1:24:A:LYS:HE2 | 12 | 0.26 |
| (1,159) | 1:24:A:LYS:HB2 | 1:24:A:LYS:HE3 | 12 | 0.26 |
| (1,159) | 1:24:A:LYS:HB3 | 1:24:A:LYS:HE2 | 12 | 0.26 |
| (1,159) | 1:24:A:LYS:HB3 | 1:24:A:LYS:HE3 | 12 | 0.26 |
| (1,86) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HD1 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HD2 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HD1 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HD2 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HD1 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HD2 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HD1 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HD2 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HD1 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HD2 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HD1 | 20 | 0.26 |
| (1,86) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HD2 | 20 | 0.26 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 19 | 0.25 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 3 | 0.25 |
| (3,29) | 1:227:C:LYS:H | 1:239:C:VAL:O | 7 | 0.25 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 8 | 0.25 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 11 | 0.25 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 15 | 0.25 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 8 | 0.25 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 19 | 0.25 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 15 | 0.25 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 19 | 0.25 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 1 | 0.25 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 11 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 4 | 0.25 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 4 | 0.25 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 3 | 0.25 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 3 | 0.25 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 7 | 0.25 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 7 | 0.25 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD1 | 15 | 0.25 |
| (1,1508) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HD2 | 15 | 0.25 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD1 | 15 | 0.25 |
| (1,1508) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HD2 | 15 | 0.25 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD1 | 15 | 0.25 |
| (1,1508) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HD2 | 15 | 0.25 |
| (1,1504) | 2:306:D:ILE:HB | 2:307:D:TYS:H | 12 | 0.25 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD2 | 6 | 0.25 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD3 | 6 | 0.25 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 4 | 0.25 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 4 | 0.25 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 19 | 0.25 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 19 | 0.25 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 18 | 0.25 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 18 | 0.25 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 18 | 0.25 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 18 | 0.25 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 18 | 0.25 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 18 | 0.25 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG21 | 11 | 0.25 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG22 | 11 | 0.25 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG23 | 11 | 0.25 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 7 | 0.25 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 7 | 0.25 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 7 | 0.25 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 7 | 0.25 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 7 | 0.25 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 7 | 0.25 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 15 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 15 | 0.25 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 15 | 0.25 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 18 | 0.25 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 18 | 0.25 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 16 | 0.25 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 16 | 0.25 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 7 | 0.25 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 7 | 0.25 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE1 | 2 | 0.25 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 7 | 0.25 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 7 | 0.25 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 16 | 0.25 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 16 | 0.25 |
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 17 | 0.24 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 2 | 0.24 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 7 | 0.24 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 9 | 0.24 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 13 | 0.24 |
| (3,34) | 1:238:C:ILE:O | 1:251:C:ILE:N | 11 | 0.24 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 1 | 0.24 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 12 | 0.24 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 20 | 0.24 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 2 | 0.24 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 12 | 0.24 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 3 | 0.24 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 4 | 0.24 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 14 | 0.24 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 9 | 0.24 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 16 | 0.24 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 6 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 9 | 0.24 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 11 | 0.24 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 14 | 0.24 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 16 | 0.24 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 5 | 0.24 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 8 | 0.24 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 7 | 0.24 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 16 | 0.24 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 19 | 0.24 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 10 | 0.24 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 6 | 0.24 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 6 | 0.24 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 17 | 0.24 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 17 | 0.24 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 9 | 0.24 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 9 | 0.24 |
| (1,1238) | 1:249:C:VAL:HG13 | 2:321:D:TYS:HE1 | 17 | 0.24 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG21 | 20 | 0.24 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG22 | 20 | 0.24 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG23 | 20 | 0.24 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 19 | 0.24 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD2 | 9 | 0.24 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD3 | 9 | 0.24 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG21 | 13 | 0.24 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG22 | 13 | 0.24 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG23 | 13 | 0.24 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 13 | 0.24 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 13 | 0.24 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 13 | 0.24 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 13 | 0.24 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 13 | 0.24 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 13 | 0.24 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 13 | 0.23 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 9 | 0.23 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 10 | 0.23 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 19 | 0.23 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 13 | 0.23 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 6 | 0.23 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 1 | 0.23 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 4 | 0.23 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 18 | 0.23 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 4 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 5 | 0.23 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 10 | 0.23 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 14 | 0.23 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 16 | 0.23 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 18 | 0.23 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 6 | 0.23 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 2 | 0.23 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 3 | 0.23 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 4 | 0.23 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 12 | 0.23 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 3 | 0.23 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 5 | 0.23 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 15 | 0.23 |
| (2,1) | 1:9:A:CYS:CB | 1:34:A:CYS:CB | 13 | 0.23 |
| (1,1573) | 2:325:D:LYS:H | 2:325:D:LYS:HG2 | 13 | 0.23 |
| (1,1573) | 2:325:D:LYS:H | 2:325:D:LYS:HG3 | 13 | 0.23 |
| (1,1504) | 2:306:D:ILE:HB | 2:307:D:TYS:H | 4 | 0.23 |
| (1,1504) | 2:306:D:ILE:HB | 2:307:D:TYS:H | 7 | 0.23 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 2 | 0.23 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 2 | 0.23 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 2 | 0.23 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 2 | 0.23 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 3 | 0.23 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 3 | 0.23 |
| (1,655) | 1:64:A:LYS:HG3 | 1:65:A:CYS:H | 5 | 0.23 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 5 | 0.23 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 5 | 0.23 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 20 | 0.23 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 20 | 0.23 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 7 | 0.23 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 7 | 0.23 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 7 | 0.23 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 7 | 0.23 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 7 | 0.23 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HD1 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HD2 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HD1 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HD2 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HD1 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HD2 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HD1 | 7 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,86) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HD2 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HD1 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HD2 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HD1 | 7 | 0.23 |
| (1,86) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HD2 | 7 | 0.23 |
| (1,64) | 1:15:A:GLU:HG2 | 2:123:B:SER:HA | 16 | 0.23 |
| (1,64) | 1:15:A:GLU:HG3 | 2:123:B:SER:HA | 16 | 0.23 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 12 | 0.22 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 3 | 0.22 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 2 | 0.22 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 19 | 0.22 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 18 | 0.22 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 16 | 0.22 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 4 | 0.22 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 8 | 0.22 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 15 | 0.22 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 1 | 0.22 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 4 | 0.22 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 10 | 0.22 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 18 | 0.22 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 20 | 0.22 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 14 | 0.22 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 5 | 0.22 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 5 | 0.22 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 16 | 0.22 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 16 | 0.22 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 17 | 0.22 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 17 | 0.22 |
| (1,1442) | 1:264:C:LYS:HG2 | 1:264:C:LYS:HE2 | 14 | 0.22 |
| (1,1442) | 1:264:C:LYS:HG2 | 1:264:C:LYS:HE3 | 14 | 0.22 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE2 | 2 | 0.22 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE3 | 2 | 0.22 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 2 | 0.22 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 2 | 0.22 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 2 | 0.22 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 2 | 0.22 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 2 | 0.22 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE1 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HE2 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE1 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HE2 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE1 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HE2 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE1 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HE2 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE1 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HE2 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE1 | 2 | 0.22 |
| (1,967) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HE2 | 2 | 0.22 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 14 | 0.22 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 3 | 0.22 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 3 | 0.22 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE2 | 16 | 0.22 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE1 | 18 | 0.22 |
| (1,412) | 1:47:A:ARG:HD2 | 2:121:B:TYS:HE2 | 18 | 0.22 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE1 | 18 | 0.22 |
| (1,412) | 1:47:A:ARG:HD3 | 2:121:B:TYS:HE2 | 18 | 0.22 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG21 | 14 | 0.22 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG22 | 14 | 0.22 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG23 | 14 | 0.22 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG21 | 16 | 0.22 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG22 | 16 | 0.22 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG23 | 16 | 0.22 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 18 | 0.22 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 18 | 0.22 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 6 | 0.21 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 15 | 0.21 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 7 | 0.21 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 20 | 0.21 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 11 | 0.21 |
| (3,33) | 1:238:C:ILE:O | 1:251:C:ILE:H | 14 | 0.21 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 8 | 0.21 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 17 | 0.21 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 11 | 0.21 |
| (3,16) | 1:28:A:ILE:O | 1:226:C:LEU:N | 1 | 0.21 |
| (3,14) | 1:28:A:ILE:N | 1:226:C:LEU:O | 15 | 0.21 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 19 | 0.21 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 4 | 0.21 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 8 | 0.21 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 11 | 0.21 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 17 | 0.21 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 14 | 0.21 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 12 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 10 | 0.21 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 15 | 0.21 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 15 | 0.21 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 15 | 0.21 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 15 | 0.21 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 14 | 0.21 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 15 | 0.21 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 18 | 0.21 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE1 | 3 | 0.21 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE2 | 3 | 0.21 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE1 | 3 | 0.21 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE2 | 3 | 0.21 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE1 | 3 | 0.21 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE2 | 3 | 0.21 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 4 | 0.21 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 4 | 0.21 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 4 | 0.21 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 4 | 0.21 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 4 | 0.21 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 4 | 0.21 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD1 | 11 | 0.21 |
| (1,1236) | 1:249:C:VAL:HB | 2:321:D:TYS:HD2 | 11 | 0.21 |
| (1,1210) | 1:242:C:LEU:HD11 | 1:249:C:VAL:HB | 16 | 0.21 |
| (1,1210) | 1:242:C:LEU:HD12 | 1:249:C:VAL:HB | 16 | 0.21 |
| (1,1210) | 1:242:C:LEU:HD13 | 1:249:C:VAL:HB | 16 | 0.21 |
| (1,1210) | 1:242:C:LEU:HD21 | 1:249:C:VAL:HB | 16 | 0.21 |
| (1,1210) | 1:242:C:LEU:HD22 | 1:249:C:VAL:HB | 16 | 0.21 |
| (1,1210) | 1:242:C:LEU:HD23 | 1:249:C:VAL:HB | 16 | 0.21 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG21 | 1 | 0.21 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG22 | 1 | 0.21 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG23 | 1 | 0.21 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE1 | 13 | 0.21 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE2 | 13 | 0.21 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE1 | 13 | 0.21 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE2 | 13 | 0.21 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG21 | 15 | 0.21 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG22 | 15 | 0.21 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG23 | 15 | 0.21 |
| (1,935) | 1:215:C:GLU:HG2 | 2:323:D:SER:HA | 5 | 0.21 |
| (1,935) | 1:215:C:GLU:HG3 | 2:323:D:SER:HA | 5 | 0.21 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 3 | 0.21 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 3 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 19 | 0.21 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 19 | 0.21 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 3 | 0.21 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 3 | 0.21 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 3 | 0.21 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 3 | 0.21 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 11 | 0.21 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 11 | 0.21 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 11 | 0.21 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 11 | 0.21 |
| (1,754) | 2:107:B:TYS:HD2 | 1:223:C:VAL:HG22 | 11 | 0.21 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 2 | 0.21 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 2 | 0.21 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 2 | 0.21 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD1 | 8 | 0.21 |
| (1,739) | 2:106:B:ILE:HB | 2:107:B:TYS:HD2 | 8 | 0.21 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 6 | 0.21 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 6 | 0.21 |
| (1,483) | 1:54:A:LYS:HB3 | 1:54:A:LYS:HE2 | 5 | 0.21 |
| (1,483) | 1:54:A:LYS:HB3 | 1:54:A:LYS:HE3 | 5 | 0.21 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG21 | 5 | 0.21 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG22 | 5 | 0.21 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG23 | 5 | 0.21 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 3 | 0.2 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 18 | 0.2 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 15 | 0.2 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 10 | 0.2 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 12 | 0.2 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 15 | 0.2 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 19 | 0.2 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 18 | 0.2 |
| (3,19) | 1:38:A:ILE:O | 1:51:A:ILE:N | 20 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 6 | 0.2 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 15 | 0.2 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 6 | 0.2 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 3 | 0.2 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 9 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD2 | 11 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD3 | 11 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD2 | 11 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD3 | 11 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD2 | 17 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD3 | 17 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD2 | 17 | 0.2 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD3 | 17 | 0.2 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 8 | 0.2 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 8 | 0.2 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE1 | 17 | 0.2 |
| (1,1515) | 2:306:D:ILE:HG21 | 2:307:D:TYS:HE2 | 17 | 0.2 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE1 | 17 | 0.2 |
| (1,1515) | 2:306:D:ILE:HG22 | 2:307:D:TYS:HE2 | 17 | 0.2 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE1 | 17 | 0.2 |
| (1,1515) | 2:306:D:ILE:HG23 | 2:307:D:TYS:HE2 | 17 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG21 | 5 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG22 | 5 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG23 | 5 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG21 | 13 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG22 | 13 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG23 | 13 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG21 | 14 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG22 | 14 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG23 | 14 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG21 | 17 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG22 | 17 | 0.2 |
| (1,1146) | 1:238:C:ILE:HB | 1:251:C:ILE:HG23 | 17 | 0.2 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE1 | 14 | 0.2 |
| (1,1112) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HE2 | 14 | 0.2 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE1 | 14 | 0.2 |
| (1,1112) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HE2 | 14 | 0.2 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE1 | 14 | 0.2 |
| (1,1112) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HE2 | 14 | 0.2 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE1 | 10 | 0.2 |
| (1,897) | 1:210:C:PRO:HG2 | 2:312:D:TYS:HE2 | 10 | 0.2 |
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE1 | 10 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,897) | 1:210:C:PRO:HG3 | 2:312:D:TYS:HE2 | 10 | 0.2 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 11 | 0.2 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 11 | 0.2 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 11 | 0.2 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 11 | 0.2 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 2 | 0.2 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 2 | 0.2 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 2 | 0.2 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 2 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 14 | 0.2 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 14 | 0.2 |
| (1,736) | 2:106:B:ILE:HA | 2:107:B:TYS:H | 13 | 0.2 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 3 | 0.2 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 11 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 11 | 0.2 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 19 | 0.2 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 19 | 0.2 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG2 | 2 | 0.2 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG3 | 2 | 0.2 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG21 | 17 | 0.2 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG22 | 17 | 0.2 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG23 | 17 | 0.2 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 9 | 0.2 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 9 | 0.2 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 9 | 0.2 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 9 | 0.2 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 9 | 0.2 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 9 | 0.2 |
| (1,167) | 1:24:A:LYS:HG2 | 1:43:A:LYS:H | 6 | 0.2 |
| (1,167) | 1:24:A:LYS:HG3 | 1:43:A:LYS:H | 6 | 0.2 |
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 12 | 0.19 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 4 | 0.19 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 9 | 0.19 |
| (3,32) | 1:227:C:LYS:O | 1:239:C:VAL:N | 10 | 0.19 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 5 | 0.19 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 18 | 0.19 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 16 | 0.19 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 17 | 0.19 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 3 | 0.19 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 20 | 0.19 |
| (3,16) | 1:28:A:ILE:O | 1:226:C:LEU:N | 3 | 0.19 |
| (3,16) | 1:28:A:ILE:O | 1:226:C:LEU:N | 16 | 0.19 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 3 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 5 | 0.19 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 8 | 0.19 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 15 | 0.19 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 14 | 0.19 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 8 | 0.19 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 18 | 0.19 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 18 | 0.19 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 18 | 0.19 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 18 | 0.19 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 4 | 0.19 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 4 | 0.19 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 10 | 0.19 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 10 | 0.19 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG2 | 2 | 0.19 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG3 | 2 | 0.19 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE2 | 19 | 0.19 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE3 | 19 | 0.19 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 3 | 0.19 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 3 | 0.19 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 3 | 0.19 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 3 | 0.19 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 3 | 0.19 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 3 | 0.19 |
| (1,1001) | 1:222:C:ASN:HB2 | 1:243:C:LYS:HD3 | 18 | 0.19 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD1 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD2 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD1 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD2 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD1 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD2 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD1 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD2 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD1 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD2 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD1 | 16 | 0.19 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD2 | 16 | 0.19 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 5 | 0.19 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 5 | 0.19 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE1 | 14 | 0.19 |
| (1,955) | 1:218:C:VAL:HB | 2:321:D:TYS:HE2 | 14 | 0.19 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 2 | 0.19 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 2 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 2 | 0.19 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 2 | 0.19 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 15 | 0.19 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 15 | 0.19 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 17 | 0.19 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 18 | 0.19 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 14 | 0.19 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 14 | 0.19 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 13 | 0.19 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 13 | 0.19 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 13 | 0.19 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 13 | 0.19 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 8 | 0.19 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 8 | 0.19 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE1 | 20 | 0.19 |
| (1,155) | 1:24:A:LYS:HB3 | 1:24:A:LYS:HE2 | 12 | 0.19 |
| (1,155) | 1:24:A:LYS:HB3 | 1:24:A:LYS:HE3 | 12 | 0.19 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 1 | 0.18 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 13 | 0.18 |
| (3,29) | 1:227:C:LYS:H | 1:239:C:VAL:O | 9 | 0.18 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 7 | 0.18 |
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 11 | 0.18 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 13 | 0.18 |
| (3,15) | 1:28:A:ILE:O | 1:226:C:LEU:H | 1 | 0.18 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 2 | 0.18 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 6 | 0.18 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 20 | 0.18 |
| (3,6) | 1:26:A:LEU:N | 1:228:C:ILE:O | 9 | 0.18 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 14 | 0.18 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 19 | 0.18 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 20 | 0.18 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 11 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 11 | 0.18 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 11 | 0.18 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 11 | 0.18 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 8 | 0.18 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 8 | 0.18 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD1 | 17 | 0.18 |
| (1,1550) | 2:320:D:ASP:HB2 | 2:321:D:TYS:HD2 | 17 | 0.18 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG2 | 10 | 0.18 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG3 | 10 | 0.18 |
| (1,1446) | 1:264:C:LYS:HG3 | 1:265:C:CYS:H | 15 | 0.18 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE2 | 5 | 0.18 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE3 | 5 | 0.18 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE2 | 17 | 0.18 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE3 | 17 | 0.18 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 5 | 0.18 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 5 | 0.18 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 5 | 0.18 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 5 | 0.18 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 5 | 0.18 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 5 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG11 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG12 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG13 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG21 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG22 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG23 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG11 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG12 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG13 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG21 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG22 | 4 | 0.18 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG23 | 4 | 0.18 |
| (1,961) | 1:218:C:VAL:HG11 | 1:252:C:ASP:H | 15 | 0.18 |
| (1,961) | 1:218:C:VAL:HG12 | 1:252:C:ASP:H | 15 | 0.18 |
| (1,961) | 1:218:C:VAL:HG13 | 1:252:C:ASP:H | 15 | 0.18 |
| (1,961) | 1:218:C:VAL:HG21 | 1:252:C:ASP:H | 15 | 0.18 |
| (1,961) | 1:218:C:VAL:HG22 | 1:252:C:ASP:H | 15 | 0.18 |
| (1,961) | 1:218:C:VAL:HG23 | 1:252:C:ASP:H | 15 | 0.18 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG21 | 9 | 0.18 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG22 | 9 | 0.18 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG23 | 9 | 0.18 |
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE1 | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,882) | 1:210:C:PRO:HA | 2:312:D:TYS:HE2 | 8 | 0.18 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 15 | 0.18 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 15 | 0.18 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 15 | 0.18 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 15 | 0.18 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 18 | 0.18 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 18 | 0.18 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 18 | 0.18 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 18 | 0.18 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 7 | 0.18 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 7 | 0.18 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 7 | 0.18 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 10 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 6 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 11 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 16 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 16 | 0.18 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 16 | 0.18 |
| (1,825) | 2:127:B:PRO:HA | 2:128:B:ALA:H | 6 | 0.18 |
| (1,691) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HB2 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HB3 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HB2 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HB3 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HB2 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HB3 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HB2 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HB3 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HB2 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HB3 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HB2 | 1 | 0.18 |
| (1,691) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HB3 | 1 | 0.18 |
| (1,681) | 1:66:A:LEU:HD21 | 1:263:C:GLU:H | 12 | 0.18 |
| (1,681) | 1:66:A:LEU:HD22 | 1:263:C:GLU:H | 12 | 0.18 |
| (1,681) | 1:66:A:LEU:HD23 | 1:263:C:GLU:H | 12 | 0.18 |
| (1,648) | 1:64:A:LYS:HB3 | 1:64:A:LYS:HE2 | 1 | 0.18 |
| (1,648) | 1:64:A:LYS:HB3 | 1:64:A:LYS:HE3 | 1 | 0.18 |
| (1,421) | 1:49:A:VAL:HG13 | 2:121:B:TYS:HE1 | 3 | 0.18 |
| (1,369) | 1:41:A:ARG:HB2 | 1:48:A:GLN:HG2 | 12 | 0.18 |
| (1,369) | 1:41:A:ARG:HB2 | 1:48:A:GLN:HG3 | 12 | 0.18 |
| (1,369) | 1:41:A:ARG:HB3 | 1:48:A:GLN:HG2 | 12 | 0.18 |
| (1,369) | 1:41:A:ARG:HB3 | 1:48:A:GLN:HG3 | 12 | 0.18 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 14 | 0.18 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 14 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 16 | 0.17 |
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 13 | 0.17 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 18 | 0.17 |
| (3,29) | 1:227:C:LYS:H | 1:239:C:VAL:O | 11 | 0.17 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 17 | 0.17 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 20 | 0.17 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 3 | 0.17 |
| (3,18) | 1:38:A:ILE:O | 1:51:A:ILE:H | 18 | 0.17 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 13 | 0.17 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 1 | 0.17 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 15 | 0.17 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 15 | 0.17 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 8 | 0.17 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 20 | 0.17 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 10 | 0.17 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 10 | 0.17 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 10 | 0.17 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 10 | 0.17 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 19 | 0.17 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 19 | 0.17 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 19 | 0.17 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 19 | 0.17 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD2 | 3 | 0.17 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD3 | 3 | 0.17 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD2 | 3 | 0.17 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD3 | 3 | 0.17 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE1 | 6 | 0.17 |
| (1,1509) | 2:306:D:ILE:HD11 | 2:307:D:TYS:HE2 | 6 | 0.17 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE1 | 6 | 0.17 |
| (1,1509) | 2:306:D:ILE:HD12 | 2:307:D:TYS:HE2 | 6 | 0.17 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE1 | 6 | 0.17 |
| (1,1509) | 2:306:D:ILE:HD13 | 2:307:D:TYS:HE2 | 6 | 0.17 |
| (1,1507) | 2:306:D:ILE:HD11 | 2:307:D:TYS:H | 19 | 0.17 |
| (1,1507) | 2:306:D:ILE:HD12 | 2:307:D:TYS:H | 19 | 0.17 |
| (1,1507) | 2:306:D:ILE:HD13 | 2:307:D:TYS:H | 19 | 0.17 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 20 | 0.17 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG2 | 14 | 0.17 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG3 | 14 | 0.17 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 1 | 0.17 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 1 | 0.17 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 5 | 0.17 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 16 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 16 | 0.17 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 16 | 0.17 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 16 | 0.17 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 16 | 0.17 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 16 | 0.17 |
| (1,1130) | 1:237:C:GLN:H | 1:253:C:PRO:HG3 | 3 | 0.17 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB2 | 10 | 0.17 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB3 | 10 | 0.17 |
| (1,1036) | 1:224:C:LYS:HG2 | 1:243:C:LYS:H | 18 | 0.17 |
| (1,1036) | 1:224:C:LYS:HG3 | 1:243:C:LYS:H | 18 | 0.17 |
| (1,1035) | 1:224:C:LYS:HG2 | 1:225:C:HIS:H | 5 | 0.17 |
| (1,1035) | 1:224:C:LYS:HG3 | 1:225:C:HIS:H | 5 | 0.17 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 19 | 0.17 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 19 | 0.17 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 19 | 0.17 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 19 | 0.17 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 4 | 0.17 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 4 | 0.17 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 8 | 0.17 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 8 | 0.17 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 17 | 0.17 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 17 | 0.17 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 7 | 0.17 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 7 | 0.17 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 6 | 0.17 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 6 | 0.17 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 6 | 0.17 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 6 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 1 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 13 | 0.17 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 13 | 0.17 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 10 | 0.17 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 10 | 0.17 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE1 | 14 | 0.17 |
| (1,743) | 2:106:B:ILE:HD11 | 2:107:B:TYS:HE2 | 14 | 0.17 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE1 | 14 | 0.17 |
| (1,743) | 2:106:B:ILE:HD12 | 2:107:B:TYS:HE2 | 14 | 0.17 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE1 | 14 | 0.17 |
| (1,743) | 2:106:B:ILE:HD13 | 2:107:B:TYS:HE2 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 14 | 0.17 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 14 | 0.17 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 4 | 0.17 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 4 | 0.17 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 11 | 0.17 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 11 | 0.17 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 11 | 0.17 |
| (1,655) | 1:64:A:LYS:HG3 | 1:65:A:CYS:H | 12 | 0.17 |
| (1,447) | 1:51:A:ILE:HG21 | 1:58:A:ILE:HG12 | 17 | 0.17 |
| (1,447) | 1:51:A:ILE:HG21 | 1:58:A:ILE:HG13 | 17 | 0.17 |
| (1,447) | 1:51:A:ILE:HG22 | 1:58:A:ILE:HG12 | 17 | 0.17 |
| (1,447) | 1:51:A:ILE:HG22 | 1:58:A:ILE:HG13 | 17 | 0.17 |
| (1,447) | 1:51:A:ILE:HG23 | 1:58:A:ILE:HG12 | 17 | 0.17 |
| (1,447) | 1:51:A:ILE:HG23 | 1:58:A:ILE:HG13 | 17 | 0.17 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 11 | 0.17 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 11 | 0.17 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 11 | 0.17 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 11 | 0.17 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 11 | 0.17 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 11 | 0.17 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 18 | 0.17 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 18 | 0.17 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 18 | 0.17 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 18 | 0.17 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 18 | 0.17 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 18 | 0.17 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG21 | 11 | 0.17 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG22 | 11 | 0.17 |
| (1,330) | 1:38:A:ILE:HB | 1:51:A:ILE:HG23 | 11 | 0.17 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 20 | 0.17 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 20 | 0.17 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 20 | 0.17 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 20 | 0.17 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 20 | 0.17 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 20 | 0.17 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 1 | 0.17 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 1 | 0.17 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 1 | 0.17 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 1 | 0.17 |
| (1,149) | 1:24:A:LYS:H | 1:43:A:LYS:HG3 | 18 | 0.17 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE1 | 10 | 0.17 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE2 | 10 | 0.17 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE1 | 10 | 0.17 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE2 | 10 | 0.17 |
| (1,69) | 1:16:A:SER:HB2 | 1:52:A:ASP:H | 13 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,69) | 1:16:A:SER:HB3 | 1:52:A:ASP:H | 13 | 0.17 |
| (1,69) | 1:16:A:SER:HB2 | 1:52:A:ASP:H | 17 | 0.17 |
| (1,69) | 1:16:A:SER:HB3 | 1:52:A:ASP:H | 17 | 0.17 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 7 | 0.16 |
| (3,30) | 1:227:C:LYS:N | 1:239:C:VAL:O | 12 | 0.16 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 10 | 0.16 |
| (3,15) | 1:28:A:ILE:O | 1:226:C:LEU:H | 3 | 0.16 |
| (3,11) | 1:27:A:LYS:O | 1:39:A:VAL:H | 15 | 0.16 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 4 | 0.16 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 4 | 0.16 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 13 | 0.16 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 13 | 0.16 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 15 | 0.16 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 15 | 0.16 |
| (1,1589) | 2:327:D:PRO:HA | 2:328:D:ALA:H | 6 | 0.16 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 15 | 0.16 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 15 | 0.16 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 18 | 0.16 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 18 | 0.16 |
| (1,1516) | 2:307:D:TYS:H | 2:307:D:TYS:HB3 | 15 | 0.16 |
| (1,1516) | 2:307:D:TYS:H | 2:307:D:TYS:HB3 | 15 | 0.16 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD2 | 9 | 0.16 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD3 | 9 | 0.16 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 1 | 0.16 |
| (1,1443) | 1:264:C:LYS:HG2 | 1:265:C:CYS:H | 7 | 0.16 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD2 | 16 | 0.16 |
| (1,1432) | 1:264:C:LYS:HA | 1:264:C:LYS:HD3 | 16 | 0.16 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 1 | 0.16 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 1 | 0.16 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 1 | 0.16 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 1 | 0.16 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 1 | 0.16 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 1 | 0.16 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HD1 | 1 | 0.16 |
| (1,1164) | 1:239:C:VAL:HG11 | 1:249:C:VAL:H | 7 | 0.16 |
| (1,1164) | 1:239:C:VAL:HG12 | 1:249:C:VAL:H | 7 | 0.16 |
| (1,1164) | 1:239:C:VAL:HG13 | 1:249:C:VAL:H | 7 | 0.16 |
| (1,1164) | 1:239:C:VAL:HG21 | 1:249:C:VAL:H | 7 | 0.16 |
| (1,1164) | 1:239:C:VAL:HG22 | 1:249:C:VAL:H | 7 | 0.16 |
| (1,1164) | 1:239:C:VAL:HG23 | 1:249:C:VAL:H | 7 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG11 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG12 | 13 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG13 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG21 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG22 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG23 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG11 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG12 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG13 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG21 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG22 | 13 | 0.16 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG23 | 13 | 0.16 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 9 | 0.16 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 9 | 0.16 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 9 | 0.16 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 9 | 0.16 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 9 | 0.16 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 9 | 0.16 |
| (1,1018) | 1:224:C:LYS:H | 1:243:C:LYS:HG3 | 18 | 0.16 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD1 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG11 | 2:321:D:TYS:HD2 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD1 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG12 | 2:321:D:TYS:HD2 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD1 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG13 | 2:321:D:TYS:HD2 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD1 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG21 | 2:321:D:TYS:HD2 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD1 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG22 | 2:321:D:TYS:HD2 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD1 | 7 | 0.16 |
| (1,966) | 1:218:C:VAL:HG23 | 2:321:D:TYS:HD2 | 7 | 0.16 |
| (1,935) | 1:215:C:GLU:HG2 | 2:323:D:SER:HA | 19 | 0.16 |
| (1,935) | 1:215:C:GLU:HG3 | 2:323:D:SER:HA | 19 | 0.16 |
| (1,857) | 2:131:B:GLU:HB2 | 2:132:B:GLU:H | 9 | 0.16 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 13 | 0.16 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 13 | 0.16 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 9 | 0.16 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 9 | 0.16 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 9 | 0.16 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 9 | 0.16 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 10 | 0.16 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 10 | 0.16 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 10 | 0.16 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 10 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE1 | 18 | 0.16 |
| (1,797) | 2:121:B:TYS:H | 2:121:B:TYS:HE2 | 18 | 0.16 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 15 | 0.16 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 15 | 0.16 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 15 | 0.16 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 15 | 0.16 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 15 | 0.16 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 15 | 0.16 |
| (1,659) | 1:65:A:CYS:H | 1:68:A:LYS:HD2 | 7 | 0.16 |
| (1,659) | 1:65:A:CYS:H | 1:68:A:LYS:HD3 | 7 | 0.16 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 4 | 0.16 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 4 | 0.16 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 4 | 0.16 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 4 | 0.16 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 4 | 0.16 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 4 | 0.16 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 16 | 0.16 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 16 | 0.16 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 16 | 0.16 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 16 | 0.16 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 16 | 0.16 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 16 | 0.16 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 6 | 0.16 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 6 | 0.16 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 6 | 0.16 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 6 | 0.16 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 6 | 0.16 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 6 | 0.16 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD1 | 10 | 0.16 |
| (1,293) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HD2 | 10 | 0.16 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD1 | 10 | 0.16 |
| (1,293) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HD2 | 10 | 0.16 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD1 | 10 | 0.16 |
| (1,293) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HD2 | 10 | 0.16 |
| (1,164) | 1:24:A:LYS:HE2 | 1:43:A:LYS:H | 5 | 0.16 |
| (1,164) | 1:24:A:LYS:HE3 | 1:43:A:LYS:H | 5 | 0.16 |
| (1,130) | 1:22:A:ASN:HB2 | 1:43:A:LYS:HD3 | 18 | 0.16 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE1 | 20 | 0.16 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE1 | 8 | 0.16 |
| (1,11) | 1:10:A:PRO:HA | 2:112:B:TYS:HE2 | 8 | 0.16 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 18 | 0.15 |
| (3,31) | 1:227:C:LYS:O | 1:239:C:VAL:H | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,27) | 1:224:C:LYS:H | 1:241:C:ARG:O | 7 | 0.15 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 11 | 0.15 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 1 | 0.15 |
| (3,12) | 1:27:A:LYS:O | 1:39:A:VAL:N | 10 | 0.15 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 1 | 0.15 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 18 | 0.15 |
| (3,6) | 1:26:A:LEU:N | 1:228:C:ILE:O | 18 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 3 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 3 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 3 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 3 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 5 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 5 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 5 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 5 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 13 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 13 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 13 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 13 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 14 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 14 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 14 | 0.15 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 14 | 0.15 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 19 | 0.15 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 19 | 0.15 |
| (1,1617) | 2:331:D:GLU:HB2 | 2:332:D:GLU:H | 9 | 0.15 |
| (1,1606) | 2:330:D:ARG:HA | 2:331:D:GLU:H | 6 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 5 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 5 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 7 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 7 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 9 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 9 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 10 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 10 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 11 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 11 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 12 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 12 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 18 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 18 | 0.15 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 19 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 19 | 0.15 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 2 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD2 | 4 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD3 | 4 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD2 | 4 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD3 | 4 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD2 | 19 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD3 | 19 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD2 | 19 | 0.15 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD3 | 19 | 0.15 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD1 | 20 | 0.15 |
| (1,1518) | 2:307:D:TYS:HA | 2:307:D:TYS:HD2 | 20 | 0.15 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 9 | 0.15 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 9 | 0.15 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD1 | 18 | 0.15 |
| (1,1505) | 2:306:D:ILE:HB | 2:307:D:TYS:HD2 | 18 | 0.15 |
| (1,1347) | 1:256:C:LYS:HD2 | 1:260:C:GLU:HG2 | 15 | 0.15 |
| (1,1347) | 1:256:C:LYS:HD3 | 1:260:C:GLU:HG2 | 15 | 0.15 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 4 | 0.15 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE2 | 12 | 0.15 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE3 | 12 | 0.15 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD1 | 10 | 0.15 |
| (1,1241) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HD2 | 10 | 0.15 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD1 | 10 | 0.15 |
| (1,1241) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HD2 | 10 | 0.15 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD1 | 10 | 0.15 |
| (1,1241) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HD2 | 10 | 0.15 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 3 | 0.15 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 3 | 0.15 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 3 | 0.15 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 3 | 0.15 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 3 | 0.15 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 3 | 0.15 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 1 | 0.15 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 1 | 0.15 |
| (1,1186) | 1:241:C:ARG:HD2 | 1:242:C:LEU:H | 13 | 0.15 |
| (1,1186) | 1:241:C:ARG:HD3 | 1:242:C:LEU:H | 13 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG11 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG12 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG13 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG21 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG22 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG23 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG11 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG12 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG13 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG21 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG22 | 7 | 0.15 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG23 | 7 | 0.15 |
| (1,1130) | 1:237:C:GLN:H | 1:253:C:PRO:HG3 | 12 | 0.15 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB2 | 5 | 0.15 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB3 | 5 | 0.15 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 4 | 0.15 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 4 | 0.15 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 8 | 0.15 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 8 | 0.15 |
| (1,960) | 1:218:C:VAL:HG11 | 1:223:C:VAL:H | 14 | 0.15 |
| (1,960) | 1:218:C:VAL:HG12 | 1:223:C:VAL:H | 14 | 0.15 |
| (1,960) | 1:218:C:VAL:HG13 | 1:223:C:VAL:H | 14 | 0.15 |
| (1,960) | 1:218:C:VAL:HG21 | 1:223:C:VAL:H | 14 | 0.15 |
| (1,960) | 1:218:C:VAL:HG22 | 1:223:C:VAL:H | 14 | 0.15 |
| (1,960) | 1:218:C:VAL:HG23 | 1:223:C:VAL:H | 14 | 0.15 |
| (1,940) | 1:216:C:SER:HB2 | 1:252:C:ASP:H | 15 | 0.15 |
| (1,940) | 1:216:C:SER:HB3 | 1:252:C:ASP:H | 15 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 3 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 3 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 3 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 3 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 5 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 5 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 5 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 5 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 13 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 13 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 13 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 13 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 14 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 14 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 14 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 14 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 20 | 0.15 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 20 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 20 | 0.15 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 20 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,854) | 2:131:B:GLU:HA | 2:131:B:GLU:HG2 | 12 | 0.15 |
| (1,854) | 2:131:B:GLU:HA | 2:131:B:GLU:HG3 | 12 | 0.15 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 1 | 0.15 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 1 | 0.15 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 6 | 0.15 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 6 | 0.15 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 16 | 0.15 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 16 | 0.15 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 4 | 0.15 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 15 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 9 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 20 | 0.15 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 20 | 0.15 |
| (1,799) | 2:121:B:TYS:HA | 2:121:B:TYS:HD1 | 11 | 0.15 |
| (1,799) | 2:121:B:TYS:HA | 2:121:B:TYS:HD2 | 11 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 7 | 0.15 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 7 | 0.15 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 18 | 0.15 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 18 | 0.15 |
| (1,738) | 2:106:B:ILE:HB | 2:107:B:TYS:H | 11 | 0.15 |
| (1,699) | 1:67:A:ASN:HA | 1:68:A:LYS:H | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 10 | 0.15 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 20 | 0.15 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 20 | 0.15 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 1 | 0.15 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 1 | 0.15 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 1 | 0.15 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 3 | 0.15 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 3 | 0.15 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 3 | 0.15 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 7 | 0.15 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 7 | 0.15 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 9 | 0.15 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 9 | 0.15 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 9 | 0.15 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG2 | 10 | 0.15 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG3 | 10 | 0.15 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG2 | 14 | 0.15 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG3 | 14 | 0.15 |
| (1,655) | 1:64:A:LYS:HG3 | 1:65:A:CYS:H | 20 | 0.15 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD2 | 16 | 0.15 |
| (1,641) | 1:64:A:LYS:HA | 1:64:A:LYS:HD3 | 16 | 0.15 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 5 | 0.15 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 14 | 0.15 |
| (1,483) | 1:54:A:LYS:HB3 | 1:54:A:LYS:HE2 | 13 | 0.15 |
| (1,483) | 1:54:A:LYS:HB3 | 1:54:A:LYS:HE3 | 13 | 0.15 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 1 | 0.15 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 1 | 0.15 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 1 | 0.15 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 1 | 0.15 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 1 | 0.15 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 1 | 0.15 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 3 | 0.15 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 3 | 0.15 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 3 | 0.15 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 3 | 0.15 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 3 | 0.15 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 3 | 0.15 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 9 | 0.15 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 9 | 0.15 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 9 | 0.15 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 9 | 0.15 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 9 | 0.15 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 9 | 0.15 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 6 | 0.15 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 6 | 0.15 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 7 | 0.15 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 7 | 0.15 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 8 | 0.15 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 8 | 0.15 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 3 | 0.15 |
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 3 | 0.15 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 11 | 0.15 |
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 16 | 0.14 |
| (3,36) | 1:240:C:ALA:N | 1:249:C:VAL:O | 8 | 0.14 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 4 | 0.14 |
| (3,35) | 1:240:C:ALA:H | 1:249:C:VAL:O | 18 | 0.14 |
| (3,29) | 1:227:C:LYS:H | 1:239:C:VAL:O | 2 | 0.14 |
| (3,29) | 1:227:C:LYS:H | 1:239:C:VAL:O | 15 | 0.14 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 18 | 0.14 |
| (3,16) | 1:28:A:ILE:O | 1:226:C:LEU:N | 7 | 0.14 |
| (3,13) | 1:28:A:ILE:H | 1:226:C:LEU:O | 17 | 0.14 |
| (3,10) | 1:27:A:LYS:N | 1:39:A:VAL:O | 5 | 0.14 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 17 | 0.14 |
| (3,5) | 1:26:A:LEU:H | 1:228:C:ILE:O | 9 | 0.14 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 2 | 0.14 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 11 | 0.14 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 15 | 0.14 |
| (2,14) | 1:209:C:CYS:CB | 1:234:C:CYS:SG | 15 | 0.14 |
| (2,2) | 1:9:A:CYS:CB | 1:34:A:CYS:SG | 7 | 0.14 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 4 | 0.14 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 4 | 0.14 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 4 | 0.14 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 4 | 0.14 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE2 | 8 | 0.14 |
| (1,1630) | 2:338:D:LYS:HB2 | 2:338:D:LYS:HE3 | 8 | 0.14 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE2 | 8 | 0.14 |
| (1,1630) | 2:338:D:LYS:HB3 | 2:338:D:LYS:HE3 | 8 | 0.14 |
| (1,1614) | 2:331:D:GLU:HA | 2:331:D:GLU:HG2 | 12 | 0.14 |
| (1,1614) | 2:331:D:GLU:HA | 2:331:D:GLU:HG3 | 12 | 0.14 |
| (1,1603) | 2:330:D:ARG:H | 2:330:D:ARG:HG2 | 6 | 0.14 |
| (1,1603) | 2:330:D:ARG:H | 2:330:D:ARG:HG3 | 6 | 0.14 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 2 | 0.14 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 2 | 0.14 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 16 | 0.14 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 16 | 0.14 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 20 | 0.14 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 20 | 0.14 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 10 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE2 | 5 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE3 | 5 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE2 | 5 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE3 | 5 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE2 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE3 | 8 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE2 | 8 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE3 | 8 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE2 | 13 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE3 | 13 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE2 | 13 | 0.14 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE3 | 13 | 0.14 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD2 | 2 | 0.14 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD3 | 2 | 0.14 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD2 | 2 | 0.14 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD3 | 2 | 0.14 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 11 | 0.14 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 11 | 0.14 |
| (1,1510) | 2:306:D:ILE:HG12 | 2:307:D:TYS:H | 16 | 0.14 |
| (1,1510) | 2:306:D:ILE:HG13 | 2:307:D:TYS:H | 16 | 0.14 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 4 | 0.14 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 15 | 0.14 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG2 | 8 | 0.14 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG3 | 8 | 0.14 |
| (1,1446) | 1:264:C:LYS:HG3 | 1:265:C:CYS:H | 5 | 0.14 |
| (1,1446) | 1:264:C:LYS:HG3 | 1:265:C:CYS:H | 12 | 0.14 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE2 | 13 | 0.14 |
| (1,1299) | 1:254:C:LYS:HB3 | 1:254:C:LYS:HE3 | 13 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG21 | 1:258:C:ILE:HG12 | 1 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG21 | 1:258:C:ILE:HG13 | 1 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG22 | 1:258:C:ILE:HG12 | 1 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG22 | 1:258:C:ILE:HG13 | 1 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG23 | 1:258:C:ILE:HG12 | 1 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG23 | 1:258:C:ILE:HG13 | 1 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG21 | 1:258:C:ILE:HG12 | 17 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG21 | 1:258:C:ILE:HG13 | 17 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG22 | 1:258:C:ILE:HG12 | 17 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG22 | 1:258:C:ILE:HG13 | 17 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG23 | 1:258:C:ILE:HG12 | 17 | 0.14 |
| (1,1263) | 1:251:C:ILE:HG23 | 1:258:C:ILE:HG13 | 17 | 0.14 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE1 | 9 | 0.14 |
| (1,1242) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HE2 | 9 | 0.14 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE1 | 9 | 0.14 |
| (1,1242) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HE2 | 9 | 0.14 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE1 | 9 | 0.14 |
| (1,1242) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HE2 | 9 | 0.14 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 19 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 19 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD11 | 1:247:C:ARG:HB2 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD11 | 1:247:C:ARG:HB3 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD12 | 1:247:C:ARG:HB2 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD12 | 1:247:C:ARG:HB3 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD13 | 1:247:C:ARG:HB2 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD13 | 1:247:C:ARG:HB3 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD21 | 1:247:C:ARG:HB2 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD21 | 1:247:C:ARG:HB3 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD22 | 1:247:C:ARG:HB2 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD22 | 1:247:C:ARG:HB3 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD23 | 1:247:C:ARG:HB2 | 14 | 0.14 |
| (1,1206) | 1:242:C:LEU:HD23 | 1:247:C:ARG:HB3 | 14 | 0.14 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD1 | 6 | 0.14 |
| (1,1114) | 1:229:C:LEU:HD21 | 2:312:D:TYS:HD2 | 6 | 0.14 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD1 | 6 | 0.14 |
| (1,1114) | 1:229:C:LEU:HD22 | 2:312:D:TYS:HD2 | 6 | 0.14 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD1 | 6 | 0.14 |
| (1,1114) | 1:229:C:LEU:HD23 | 2:312:D:TYS:HD2 | 6 | 0.14 |
| (1,940) | 1:216:C:SER:HB2 | 1:252:C:ASP:H | 17 | 0.14 |
| (1,940) | 1:216:C:SER:HB3 | 1:252:C:ASP:H | 17 | 0.14 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 8 | 0.14 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 8 | 0.14 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 8 | 0.14 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 8 | 0.14 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 10 | 0.14 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 10 | 0.14 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 10 | 0.14 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 10 | 0.14 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG2 | 4 | 0.14 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG3 | 4 | 0.14 |
| (1,862) | 2:132:B:GLU:H | 2:132:B:GLU:HG2 | 6 | 0.14 |
| (1,862) | 2:132:B:GLU:H | 2:132:B:GLU:HG3 | 6 | 0.14 |
| (1,862) | 2:132:B:GLU:H | 2:132:B:GLU:HG2 | 7 | 0.14 |
| (1,862) | 2:132:B:GLU:H | 2:132:B:GLU:HG3 | 7 | 0.14 |
| (1,843) | 2:130:B:ARG:H | 2:130:B:ARG:HG2 | 12 | 0.14 |
| (1,843) | 2:130:B:ARG:H | 2:130:B:ARG:HG3 | 12 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 2 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 2 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 9 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 9 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 10 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 11 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 11 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 12 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 12 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 14 | 0.14 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 14 | 0.14 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 9 | 0.14 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 15 | 0.14 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 15 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD11 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD12 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD13 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD21 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD22 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD23 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD11 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD12 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD13 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD21 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD22 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD23 | 1 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD11 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD12 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD13 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD21 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD22 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD23 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD11 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD12 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD13 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD21 | 16 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD22 | 16 | 0.14 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD23 | 16 | 0.14 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 16 | 0.14 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 16 | 0.14 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE2 | 16 | 0.14 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE3 | 16 | 0.14 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 17 | 0.14 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 17 | 0.14 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE2 | 17 | 0.14 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE3 | 17 | 0.14 |
| (1,764) | 2:112:B:TYS:HD1 | 2:113:B:THR:H | 13 | 0.14 |
| (1,764) | 2:112:B:TYS:HD2 | 2:113:B:THR:H | 13 | 0.14 |
| (1,762) | 2:112:B:TYS:HA | 2:112:B:TYS:HD1 | 1 | 0.14 |
| (1,762) | 2:112:B:TYS:HA | 2:112:B:TYS:HD2 | 1 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 20 | 0.14 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 20 | 0.14 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD1 | 17 | 0.14 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD2 | 17 | 0.14 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD1 | 17 | 0.14 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD2 | 17 | 0.14 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD1 | 17 | 0.14 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD2 | 17 | 0.14 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 9 | 0.14 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 9 | 0.14 |
| (1,699) | 1:67:A:ASN:HA | 1:68:A:LYS:H | 11 | 0.14 |
| (1,699) | 1:67:A:ASN:HA | 1:68:A:LYS:H | 15 | 0.14 |
| (1,694) | 1:66:A:LEU:HD11 | 2:329:D:PHE:HD1 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD11 | 2:329:D:PHE:HD2 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD12 | 2:329:D:PHE:HD1 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD12 | 2:329:D:PHE:HD2 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD13 | 2:329:D:PHE:HD1 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD13 | 2:329:D:PHE:HD2 | 3 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,694) | 1:66:A:LEU:HD21 | 2:329:D:PHE:HD1 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD21 | 2:329:D:PHE:HD2 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD22 | 2:329:D:PHE:HD1 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD22 | 2:329:D:PHE:HD2 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD23 | 2:329:D:PHE:HD1 | 3 | 0.14 |
| (1,694) | 1:66:A:LEU:HD23 | 2:329:D:PHE:HD2 | 3 | 0.14 |
| (1,691) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HB2 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HB3 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HB2 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HB3 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HB2 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HB3 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HB2 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HB3 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HB2 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HB3 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HB2 | 15 | 0.14 |
| (1,691) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HB3 | 15 | 0.14 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 6 | 0.14 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 6 | 0.14 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 6 | 0.14 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 13 | 0.14 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 13 | 0.14 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 13 | 0.14 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 18 | 0.14 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 18 | 0.14 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 18 | 0.14 |
| (1,634) | 1:63:A:GLU:HG3 | 1:266:C:LEU:HG | 20 | 0.14 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 4 | 0.14 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 16 | 0.14 |
| (1,447) | 1:51:A:ILE:HG21 | 1:58:A:ILE:HG12 | 13 | 0.14 |
| (1,447) | 1:51:A:ILE:HG21 | 1:58:A:ILE:HG13 | 13 | 0.14 |
| (1,447) | 1:51:A:ILE:HG22 | 1:58:A:ILE:HG12 | 13 | 0.14 |
| (1,447) | 1:51:A:ILE:HG22 | 1:58:A:ILE:HG13 | 13 | 0.14 |
| (1,447) | 1:51:A:ILE:HG23 | 1:58:A:ILE:HG12 | 13 | 0.14 |
| (1,447) | 1:51:A:ILE:HG23 | 1:58:A:ILE:HG13 | 13 | 0.14 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD1 | 14 | 0.14 |
| (1,424) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HD2 | 14 | 0.14 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD1 | 14 | 0.14 |
| (1,424) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HD2 | 14 | 0.14 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD1 | 14 | 0.14 |
| (1,424) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HD2 | 14 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 7 | 0.14 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 7 | 0.14 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 7 | 0.14 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 7 | 0.14 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 7 | 0.14 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 7 | 0.14 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD1 | 3 | 0.14 |
| (1,419) | 1:49:A:VAL:HB | 2:121:B:TYS:HD2 | 3 | 0.14 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD2 | 8 | 0.14 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD3 | 8 | 0.14 |
| (1,295) | 1:29:A:LEU:HD21 | 1:225:C:HIS:HE1 | 13 | 0.14 |
| (1,295) | 1:29:A:LEU:HD22 | 1:225:C:HIS:HE1 | 13 | 0.14 |
| (1,295) | 1:29:A:LEU:HD23 | 1:225:C:HIS:HE1 | 13 | 0.14 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 9 | 0.14 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 9 | 0.14 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 9 | 0.14 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 9 | 0.14 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 9 | 0.14 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 9 | 0.14 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE1 | 19 | 0.14 |
| (1,290) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HE2 | 19 | 0.14 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE1 | 19 | 0.14 |
| (1,290) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HE2 | 19 | 0.14 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE1 | 19 | 0.14 |
| (1,290) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HE2 | 19 | 0.14 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 19 | 0.14 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 19 | 0.14 |
| (1,182) | 1:25:A:HIS:HE1 | 1:227:C:LYS:HE2 | 2 | 0.14 |
| (1,182) | 1:25:A:HIS:HE1 | 1:227:C:LYS:HE3 | 2 | 0.14 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 18 | 0.14 |
| (1,64) | 1:15:A:GLU:HG2 | 2:123:B:SER:HA | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,64) | 1:15:A:GLU:HG3 | 2:123:B:SER:HA | 12 | 0.14 |
| (1,64) | 1:15:A:GLU:HG2 | 2:123:B:SER:HA | 13 | 0.14 |
| (1,64) | 1:15:A:GLU:HG3 | 2:123:B:SER:HA | 13 | 0.14 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 2 | 0.13 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 8 | 0.13 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 7 | 0.13 |
| (3,15) | 1:28:A:ILE:O | 1:226:C:LEU:H | 16 | 0.13 |
| (3,7) | 1:26:A:LEU:O | 1:228:C:ILE:H | 9 | 0.13 |
| (3,6) | 1:26:A:LEU:N | 1:228:C:ILE:O | 15 | 0.13 |
| (3,4) | 1:24:A:LYS:N | 1:41:A:ARG:O | 7 | 0.13 |
| (2,14) | 1:209:C:CYS:CB | 1:234:C:CYS:SG | 4 | 0.13 |
| (2,14) | 1:209:C:CYS:CB | 1:234:C:CYS:SG | 16 | 0.13 |
| (2,10) | 1:65:A:CYS:CB | 1:236:C:CYS:CB | 7 | 0.13 |
| (2,2) | 1:9:A:CYS:CB | 1:34:A:CYS:SG | 18 | 0.13 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 9 | 0.13 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 9 | 0.13 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 17 | 0.13 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 17 | 0.13 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 1 | 0.13 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 1 | 0.13 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 6 | 0.13 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 6 | 0.13 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 14 | 0.13 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 14 | 0.13 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 7 | 0.13 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB2 | 1 | 0.13 |
| (1,1565) | 2:321:D:TYS:HD1 | 2:322:D:ASP:HB3 | 1 | 0.13 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB2 | 1 | 0.13 |
| (1,1565) | 2:321:D:TYS:HD2 | 2:322:D:ASP:HB3 | 1 | 0.13 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD1 | 7 | 0.13 |
| (1,1563) | 2:321:D:TYS:HA | 2:321:D:TYS:HD2 | 7 | 0.13 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE1 | 19 | 0.13 |
| (1,1561) | 2:321:D:TYS:H | 2:321:D:TYS:HE2 | 19 | 0.13 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD2 | 5 | 0.13 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD3 | 5 | 0.13 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD2 | 19 | 0.13 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD3 | 19 | 0.13 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 17 | 0.13 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG2 | 7 | 0.13 |
| (1,1451) | 1:265:C:CYS:H | 1:268:C:LYS:HG3 | 7 | 0.13 |
| (1,1446) | 1:264:C:LYS:HG3 | 1:265:C:CYS:H | 11 | 0.13 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 7 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1263) | 1:251:C:ILE:HG21 | 1:258:C:ILE:HG12 | 20 | 0.13 |
| (1,1263) | 1:251:C:ILE:HG21 | 1:258:C:ILE:HG13 | 20 | 0.13 |
| (1,1263) | 1:251:C:ILE:HG22 | 1:258:C:ILE:HG12 | 20 | 0.13 |
| (1,1263) | 1:251:C:ILE:HG22 | 1:258:C:ILE:HG13 | 20 | 0.13 |
| (1,1263) | 1:251:C:ILE:HG23 | 1:258:C:ILE:HG12 | 20 | 0.13 |
| (1,1263) | 1:251:C:ILE:HG23 | 1:258:C:ILE:HG13 | 20 | 0.13 |
| (1,1238) | 1:249:C:VAL:HG11 | 2:321:D:TYS:HE1 | 12 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 8 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 8 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 16 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 16 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 17 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 17 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 18 | 0.13 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 18 | 0.13 |
| (1,1157) | 1:238:C:ILE:HG21 | 1:251:C:ILE:HB | 1 | 0.13 |
| (1,1157) | 1:238:C:ILE:HG22 | 1:251:C:ILE:HB | 1 | 0.13 |
| (1,1157) | 1:238:C:ILE:HG23 | 1:251:C:ILE:HB | 1 | 0.13 |
| (1,1045) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HG2 | 7 | 0.13 |
| (1,1045) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HG3 | 7 | 0.13 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 2 | 0.13 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 2 | 0.13 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 15 | 0.13 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 15 | 0.13 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 20 | 0.13 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 20 | 0.13 |
| (1,1035) | 1:224:C:LYS:HG2 | 1:225:C:HIS:H | 14 | 0.13 |
| (1,1035) | 1:224:C:LYS:HG3 | 1:225:C:HIS:H | 14 | 0.13 |
| (1,1035) | 1:224:C:LYS:HG2 | 1:225:C:HIS:H | 17 | 0.13 |
| (1,1035) | 1:224:C:LYS:HG3 | 1:225:C:HIS:H | 17 | 0.13 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG21 | 16 | 0.13 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG22 | 16 | 0.13 |
| (1,951) | 1:218:C:VAL:HB | 1:251:C:ILE:HG23 | 16 | 0.13 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD11 | 17 | 0.13 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD12 | 17 | 0.13 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD13 | 17 | 0.13 |
| (1,885) | 1:210:C:PRO:HB2 | 2:312:D:TYS:HE2 | 6 | 0.13 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE2 | 4 | 0.13 |
| (1,870) | 2:138:B:LYS:HB2 | 2:138:B:LYS:HE3 | 4 | 0.13 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE2 | 4 | 0.13 |
| (1,870) | 2:138:B:LYS:HB3 | 2:138:B:LYS:HE3 | 4 | 0.13 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 13 | 0.13 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 14 | 0.13 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 14 | 0.13 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 5 | 0.13 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 5 | 0.13 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 20 | 0.13 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 20 | 0.13 |
| (1,830) | 2:127:B:PRO:HG2 | 2:128:B:ALA:H | 4 | 0.13 |
| (1,830) | 2:127:B:PRO:HG3 | 2:128:B:ALA:H | 4 | 0.13 |
| (1,830) | 2:127:B:PRO:HG2 | 2:128:B:ALA:H | 9 | 0.13 |
| (1,830) | 2:127:B:PRO:HG3 | 2:128:B:ALA:H | 9 | 0.13 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 18 | 0.13 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 18 | 0.13 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE2 | 18 | 0.13 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE3 | 18 | 0.13 |
| (1,808) | 2:125:B:LYS:H | 2:125:B:LYS:HD2 | 7 | 0.13 |
| (1,808) | 2:125:B:LYS:H | 2:125:B:LYS:HD3 | 7 | 0.13 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 8 | 0.13 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 8 | 0.13 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 8 | 0.13 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 8 | 0.13 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 10 | 0.13 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 10 | 0.13 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD1 | 6 | 0.13 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD2 | 6 | 0.13 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD1 | 6 | 0.13 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD2 | 6 | 0.13 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD1 | 6 | 0.13 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD2 | 6 | 0.13 |
| (1,747) | 2:106:B:ILE:HG21 | 2:107:B:TYS:H | 5 | 0.13 |
| (1,747) | 2:106:B:ILE:HG22 | 2:107:B:TYS:H | 5 | 0.13 |
| (1,747) | 2:106:B:ILE:HG23 | 2:107:B:TYS:H | 5 | 0.13 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 4 | 0.13 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 4 | 0.13 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 4 | 0.13 |
| (1,741) | 2:106:B:ILE:HD11 | 2:107:B:TYS:H | 7 | 0.13 |
| (1,741) | 2:106:B:ILE:HD12 | 2:107:B:TYS:H | 7 | 0.13 |
| (1,741) | 2:106:B:ILE:HD13 | 2:107:B:TYS:H | 7 | 0.13 |
| (1,701) | 1:67:A:ASN:HB2 | 1:68:A:LYS:HB2 | 19 | 0.13 |
| (1,701) | 1:67:A:ASN:HB2 | 1:68:A:LYS:HB3 | 19 | 0.13 |
| (1,701) | 1:67:A:ASN:HB3 | 1:68:A:LYS:HB2 | 19 | 0.13 |
| (1,701) | 1:67:A:ASN:HB3 | 1:68:A:LYS:HB3 | 19 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,699) | 1:67:A:ASN:HA | 1:68:A:LYS:H | 4 | 0.13 |
| (1,699) | 1:67:A:ASN:HA | 1:68:A:LYS:H | 16 | 0.13 |
| (1,691) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HB2 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HB3 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HB2 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HB3 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HB2 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HB3 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HB2 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HB3 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HB2 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HB3 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HB2 | 13 | 0.13 |
| (1,691) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HB3 | 13 | 0.13 |
| (1,681) | 1:66:A:LEU:HD21 | 1:263:C:GLU:H | 14 | 0.13 |
| (1,681) | 1:66:A:LEU:HD22 | 1:263:C:GLU:H | 14 | 0.13 |
| (1,681) | 1:66:A:LEU:HD23 | 1:263:C:GLU:H | 14 | 0.13 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 19 | 0.13 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 19 | 0.13 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 19 | 0.13 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG2 | 8 | 0.13 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG3 | 8 | 0.13 |
| (1,648) | 1:64:A:LYS:HB3 | 1:64:A:LYS:HE2 | 14 | 0.13 |
| (1,648) | 1:64:A:LYS:HB3 | 1:64:A:LYS:HE3 | 14 | 0.13 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 1 | 0.13 |
| (1,428) | 1:51:A:ILE:H | 1:51:A:ILE:HD11 | 6 | 0.13 |
| (1,428) | 1:51:A:ILE:H | 1:51:A:ILE:HD12 | 6 | 0.13 |
| (1,428) | 1:51:A:ILE:H | 1:51:A:ILE:HD13 | 6 | 0.13 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 13 | 0.13 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 13 | 0.13 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 13 | 0.13 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 13 | 0.13 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 13 | 0.13 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 13 | 0.13 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD2 | 4 | 0.13 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD3 | 4 | 0.13 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD2 | 18 | 0.13 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD3 | 18 | 0.13 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD2 | 19 | 0.13 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD3 | 19 | 0.13 |
| (1,314) | 1:37:A:GLN:H | 1:53:A:PRO:HG3 | 9 | 0.13 |
| (1,295) | 1:29:A:LEU:HD21 | 1:225:C:HIS:HE1 | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,295) | 1:29:A:LEU:HD22 | 1:225:C:HIS:HE1 | 4 | 0.13 |
| (1,295) | 1:29:A:LEU:HD23 | 1:225:C:HIS:HE1 | 4 | 0.13 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE1 | 18 | 0.13 |
| (1,294) | 1:29:A:LEU:HD21 | 2:112:B:TYS:HE2 | 18 | 0.13 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE1 | 18 | 0.13 |
| (1,294) | 1:29:A:LEU:HD22 | 2:112:B:TYS:HE2 | 18 | 0.13 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE1 | 18 | 0.13 |
| (1,294) | 1:29:A:LEU:HD23 | 2:112:B:TYS:HE2 | 18 | 0.13 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD1 | 10 | 0.13 |
| (1,289) | 1:29:A:LEU:HD11 | 2:112:B:TYS:HD2 | 10 | 0.13 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD1 | 10 | 0.13 |
| (1,289) | 1:29:A:LEU:HD12 | 2:112:B:TYS:HD2 | 10 | 0.13 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD1 | 10 | 0.13 |
| (1,289) | 1:29:A:LEU:HD13 | 2:112:B:TYS:HD2 | 10 | 0.13 |
| (1,247) | 1:27:A:LYS:HE2 | 1:225:C:HIS:HD2 | 5 | 0.13 |
| (1,247) | 1:27:A:LYS:HE3 | 1:225:C:HIS:HD2 | 5 | 0.13 |
| (1,205) | 1:26:A:LEU:HD21 | 1:228:C:ILE:H | 7 | 0.13 |
| (1,205) | 1:26:A:LEU:HD22 | 1:228:C:ILE:H | 7 | 0.13 |
| (1,205) | 1:26:A:LEU:HD23 | 1:228:C:ILE:H | 7 | 0.13 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 11 | 0.13 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 11 | 0.13 |
| (1,182) | 1:25:A:HIS:HE1 | 1:227:C:LYS:HE2 | 3 | 0.13 |
| (1,182) | 1:25:A:HIS:HE1 | 1:227:C:LYS:HE3 | 3 | 0.13 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 13 | 0.13 |
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 13 | 0.13 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 14 | 0.13 |
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 14 | 0.13 |
| (1,136) | 1:23:A:VAL:HB | 1:42:A:LEU:H | 18 | 0.13 |
| (1,113) | 1:20:A:ARG:HD2 | 1:23:A:VAL:H | 12 | 0.13 |
| (1,113) | 1:20:A:ARG:HD3 | 1:23:A:VAL:H | 12 | 0.13 |
| (1,92) | 1:18:A:VAL:HG11 | 1:23:A:VAL:H | 19 | 0.13 |
| (1,92) | 1:18:A:VAL:HG12 | 1:23:A:VAL:H | 19 | 0.13 |
| (1,92) | 1:18:A:VAL:HG13 | 1:23:A:VAL:H | 19 | 0.13 |
| (1,92) | 1:18:A:VAL:HG21 | 1:23:A:VAL:H | 19 | 0.13 |
| (1,92) | 1:18:A:VAL:HG22 | 1:23:A:VAL:H | 19 | 0.13 |
| (1,92) | 1:18:A:VAL:HG23 | 1:23:A:VAL:H | 19 | 0.13 |
| (1,82) | 1:18:A:VAL:HB | 1:51:A:ILE:HG21 | 19 | 0.13 |
| (1,82) | 1:18:A:VAL:HB | 1:51:A:ILE:HG22 | 19 | 0.13 |
| (1,82) | 1:18:A:VAL:HB | 1:51:A:ILE:HG23 | 19 | 0.13 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD11 | 12 | 0.13 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD12 | 12 | 0.13 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD13 | 12 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 15 | 0.12 |
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 18 | 0.12 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 1 | 0.12 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 5 | 0.12 |
| (3,21) | 1:40:A:ALA:N | 1:49:A:VAL:O | 10 | 0.12 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 4 | 0.12 |
| (2,17) | 1:211:C:CYS:CB | 1:250:C:CYS:SG | 2 | 0.12 |
| (2,15) | 1:209:C:CYS:SG | 1:234:C:CYS:CB | 15 | 0.12 |
| (2,14) | 1:209:C:CYS:CB | 1:234:C:CYS:SG | 13 | 0.12 |
| (2,14) | 1:209:C:CYS:CB | 1:234:C:CYS:SG | 14 | 0.12 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 16 | 0.12 |
| (2,5) | 1:11:A:CYS:CB | 1:50:A:CYS:SG | 6 | 0.12 |
| (2,3) | 1:9:A:CYS:SG | 1:34:A:CYS:CB | 7 | 0.12 |
| (2,2) | 1:9:A:CYS:CB | 1:34:A:CYS:SG | 15 | 0.12 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 6 | 0.12 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 6 | 0.12 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE2 | 14 | 0.12 |
| (1,1583) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE3 | 14 | 0.12 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE2 | 14 | 0.12 |
| (1,1583) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HE3 | 14 | 0.12 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD2 | 10 | 0.12 |
| (1,1582) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HD3 | 10 | 0.12 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD2 | 10 | 0.12 |
| (1,1582) | 2:325:D:LYS:HB3 | 2:325:D:LYS:HD3 | 10 | 0.12 |
| (1,1544) | 2:315:D:GLU:HA | 2:316:D:MET:H | 11 | 0.12 |
| (1,1543) | 2:315:D:GLU:HA | 2:315:D:GLU:HG2 | 8 | 0.12 |
| (1,1543) | 2:315:D:GLU:HA | 2:315:D:GLU:HG3 | 8 | 0.12 |
| (1,1537) | 2:314:D:GLU:H | 2:314:D:GLU:HG2 | 5 | 0.12 |
| (1,1537) | 2:314:D:GLU:H | 2:314:D:GLU:HG3 | 5 | 0.12 |
| (1,1533) | 2:313:D:THR:HA | 2:314:D:GLU:H | 4 | 0.12 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 12 | 0.12 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 12 | 0.12 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 12 | 0.12 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 17 | 0.12 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 17 | 0.12 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 17 | 0.12 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD11 | 19 | 0.12 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD12 | 19 | 0.12 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD13 | 19 | 0.12 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD11 | 20 | 0.12 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD12 | 20 | 0.12 |
| (1,1500) | 2:306:D:ILE:HA | 2:306:D:ILE:HD13 | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD2 | 12 | 0.12 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD3 | 12 | 0.12 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 9 | 0.12 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 11 | 0.12 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 16 | 0.12 |
| (1,1446) | 1:264:C:LYS:HG3 | 1:265:C:CYS:H | 18 | 0.12 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 11 | 0.12 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 13 | 0.12 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 14 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 8 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 8 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 8 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 8 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 8 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 8 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 14 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 14 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 14 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 14 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 14 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 14 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 19 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 19 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 19 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 19 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 19 | 0.12 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 19 | 0.12 |
| (1,1157) | 1:238:C:ILE:HG21 | 1:251:C:ILE:HB | 14 | 0.12 |
| (1,1157) | 1:238:C:ILE:HG22 | 1:251:C:ILE:HB | 14 | 0.12 |
| (1,1157) | 1:238:C:ILE:HG23 | 1:251:C:ILE:HB | 14 | 0.12 |
| (1,1134) | 1:237:C:GLN:HE21 | 1:253:C:PRO:HG3 | 19 | 0.12 |
| (1,1134) | 1:237:C:GLN:HE22 | 1:253:C:PRO:HG3 | 19 | 0.12 |
| (1,1130) | 1:237:C:GLN:H | 1:253:C:PRO:HG3 | 5 | 0.12 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD1 | 16 | 0.12 |
| (1,1111) | 1:229:C:LEU:HD11 | 2:312:D:TYS:HD2 | 16 | 0.12 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD1 | 16 | 0.12 |
| (1,1111) | 1:229:C:LEU:HD12 | 2:312:D:TYS:HD2 | 16 | 0.12 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD1 | 16 | 0.12 |
| (1,1111) | 1:229:C:LEU:HD13 | 2:312:D:TYS:HD2 | 16 | 0.12 |
| (1,1107) | 1:229:C:LEU:HA | 1:237:C:GLN:HB2 | 19 | 0.12 |
| (1,1107) | 1:229:C:LEU:HA | 1:237:C:GLN:HB3 | 19 | 0.12 |
| (1,1045) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HG2 | 3 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1045) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HG3 | 3 | 0.12 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 9 | 0.12 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 9 | 0.12 |
| (1,1035) | 1:224:C:LYS:HG2 | 1:225:C:HIS:H | 12 | 0.12 |
| (1,1035) | 1:224:C:LYS:HG3 | 1:225:C:HIS:H | 12 | 0.12 |
| (1,1014) | 1:224:C:LYS:H | 1:224:C:LYS:HD2 | 6 | 0.12 |
| (1,1014) | 1:224:C:LYS:H | 1:224:C:LYS:HD3 | 6 | 0.12 |
| (1,1007) | 1:223:C:VAL:HB | 1:242:C:LEU:H | 18 | 0.12 |
| (1,984) | 1:220:C:ARG:HD2 | 1:223:C:VAL:H | 7 | 0.12 |
| (1,984) | 1:220:C:ARG:HD3 | 1:223:C:VAL:H | 7 | 0.12 |
| (1,935) | 1:215:C:GLU:HG2 | 2:323:D:SER:HA | 12 | 0.12 |
| (1,935) | 1:215:C:GLU:HG3 | 2:323:D:SER:HA | 12 | 0.12 |
| (1,903) | 1:212:C:ARG:HD2 | 1:213:C:PHE:HE1 | 8 | 0.12 |
| (1,903) | 1:212:C:ARG:HD2 | 1:213:C:PHE:HE2 | 8 | 0.12 |
| (1,903) | 1:212:C:ARG:HD3 | 1:213:C:PHE:HE1 | 8 | 0.12 |
| (1,903) | 1:212:C:ARG:HD3 | 1:213:C:PHE:HE2 | 8 | 0.12 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 4 | 0.12 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 4 | 0.12 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 9 | 0.12 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 9 | 0.12 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 18 | 0.12 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 18 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 1 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 2 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 13 | 0.12 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 13 | 0.12 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 5 | 0.12 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 5 | 0.12 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE2 | 5 | 0.12 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE3 | 5 | 0.12 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 8 | 0.12 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 8 | 0.12 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE2 | 8 | 0.12 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE3 | 8 | 0.12 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 14 | 0.12 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 14 | 0.12 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE2 | 14 | 0.12 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE3 | 14 | 0.12 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 4 | 0.12 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 4 | 0.12 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 4 | 0.12 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 4 | 0.12 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD2 | 19 | 0.12 |
| (1,818) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HD3 | 19 | 0.12 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD2 | 19 | 0.12 |
| (1,818) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HD3 | 19 | 0.12 |
| (1,815) | 2:125:B:LYS:HB2 | 2:126:B:GLU:H | 6 | 0.12 |
| (1,814) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 17 | 0.12 |
| (1,814) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 17 | 0.12 |
| (1,809) | 2:125:B:LYS:H | 2:125:B:LYS:HG2 | 18 | 0.12 |
| (1,809) | 2:125:B:LYS:H | 2:125:B:LYS:HG3 | 18 | 0.12 |
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE1 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,791) | 2:120:B:ASP:HB3 | 2:121:B:TYS:HE2 | 6 | 0.12 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD1 | 5 | 0.12 |
| (1,786) | 2:120:B:ASP:HB2 | 2:121:B:TYS:HD2 | 5 | 0.12 |
| (1,780) | 2:115:B:GLU:HA | 2:116:B:MET:H | 11 | 0.12 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 13 | 0.12 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 13 | 0.12 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 13 | 0.12 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 19 | 0.12 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 19 | 0.12 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 19 | 0.12 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 12 | 0.12 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 12 | 0.12 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 1 | 0.12 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 1 | 0.12 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 13 | 0.12 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 13 | 0.12 |
| (1,699) | 1:67:A:ASN:HA | 1:68:A:LYS:H | 1 | 0.12 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 2 | 0.12 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 2 | 0.12 |
| (1,679) | 1:66:A:LEU:HD11 | 1:263:C:GLU:H | 17 | 0.12 |
| (1,679) | 1:66:A:LEU:HD12 | 1:263:C:GLU:H | 17 | 0.12 |
| (1,679) | 1:66:A:LEU:HD13 | 1:263:C:GLU:H | 17 | 0.12 |
| (1,675) | 1:66:A:LEU:HG | 1:259:C:GLN:HE22 | 4 | 0.12 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG2 | 18 | 0.12 |
| (1,660) | 1:65:A:CYS:H | 1:68:A:LYS:HG3 | 18 | 0.12 |
| (1,655) | 1:64:A:LYS:HG3 | 1:65:A:CYS:H | 18 | 0.12 |
| (1,483) | 1:54:A:LYS:HB3 | 1:54:A:LYS:HE2 | 1 | 0.12 |
| (1,483) | 1:54:A:LYS:HB3 | 1:54:A:LYS:HE3 | 1 | 0.12 |
| (1,453) | 1:52:A:ASP:HB2 | 1:55:A:LEU:H | 10 | 0.12 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 19 | 0.12 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 19 | 0.12 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 19 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 19 | 0.12 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 19 | 0.12 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 19 | 0.12 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD2 | 16 | 0.12 |
| (1,406) | 1:47:A:ARG:HA | 1:47:A:ARG:HD3 | 16 | 0.12 |
| (1,391) | 1:42:A:LEU:HD11 | 1:47:A:ARG:HD2 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD11 | 1:47:A:ARG:HD3 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD12 | 1:47:A:ARG:HD2 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD12 | 1:47:A:ARG:HD3 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD13 | 1:47:A:ARG:HD2 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD13 | 1:47:A:ARG:HD3 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD21 | 1:47:A:ARG:HD2 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD21 | 1:47:A:ARG:HD3 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD22 | 1:47:A:ARG:HD2 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD22 | 1:47:A:ARG:HD3 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD23 | 1:47:A:ARG:HD2 | 20 | 0.12 |
| (1,391) | 1:42:A:LEU:HD23 | 1:47:A:ARG:HD3 | 20 | 0.12 |
| (1,341) | 1:38:A:ILE:HG21 | 1:51:A:ILE:HB | 14 | 0.12 |
| (1,341) | 1:38:A:ILE:HG22 | 1:51:A:ILE:HB | 14 | 0.12 |
| (1,341) | 1:38:A:ILE:HG23 | 1:51:A:ILE:HB | 14 | 0.12 |
| (1,341) | 1:38:A:ILE:HG21 | 1:51:A:ILE:HB | 20 | 0.12 |
| (1,341) | 1:38:A:ILE:HG22 | 1:51:A:ILE:HB | 20 | 0.12 |
| (1,341) | 1:38:A:ILE:HG23 | 1:51:A:ILE:HB | 20 | 0.12 |
| (1,248) | 1:27:A:LYS:HE2 | 1:225:C:HIS:HE1 | 18 | 0.12 |
| (1,248) | 1:27:A:LYS:HE3 | 1:225:C:HIS:HE1 | 18 | 0.12 |
| (1,187) | 1:25:A:HIS:HE1 | 1:41:A:ARG:HG2 | 2 | 0.12 |
| (1,187) | 1:25:A:HIS:HE1 | 1:41:A:ARG:HG3 | 2 | 0.12 |
| (1,187) | 1:25:A:HIS:HE1 | 1:41:A:ARG:HG2 | 15 | 0.12 |
| (1,187) | 1:25:A:HIS:HE1 | 1:41:A:ARG:HG3 | 15 | 0.12 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 16 | 0.12 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 16 | 0.12 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE2 | 20 | 0.12 |
| (1,184) | 1:25:A:HIS:HE1 | 1:27:A:LYS:HE3 | 20 | 0.12 |
| (1,167) | 1:24:A:LYS:HG2 | 1:43:A:LYS:H | 18 | 0.12 |
| (1,167) | 1:24:A:LYS:HG3 | 1:43:A:LYS:H | 18 | 0.12 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 7 | 0.12 |
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 7 | 0.12 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 1 | 0.12 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 9 | 0.12 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 12 | 0.12 |
| (1,136) | 1:23:A:VAL:HB | 1:42:A:LEU:H | 12 | 0.12 |
| (1,93) | 1:18:A:VAL:HG11 | 1:52:A:ASP:H | 16 | 0.12 |
| (1,93) | 1:18:A:VAL:HG12 | 1:52:A:ASP:H | 16 | 0.12 |
| (1,93) | 1:18:A:VAL:HG13 | 1:52:A:ASP:H | 16 | 0.12 |
| (1,93) | 1:18:A:VAL:HG21 | 1:52:A:ASP:H | 16 | 0.12 |
| (1,93) | 1:18:A:VAL:HG22 | 1:52:A:ASP:H | 16 | 0.12 |
| (1,93) | 1:18:A:VAL:HG23 | 1:52:A:ASP:H | 16 | 0.12 |
| (1,92) | 1:18:A:VAL:HG11 | 1:23:A:VAL:H | 20 | 0.12 |
| (1,92) | 1:18:A:VAL:HG12 | 1:23:A:VAL:H | 20 | 0.12 |
| (1,92) | 1:18:A:VAL:HG13 | 1:23:A:VAL:H | 20 | 0.12 |
| (1,92) | 1:18:A:VAL:HG21 | 1:23:A:VAL:H | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,92) | 1:18:A:VAL:HG22 | 1:23:A:VAL:H | 20 | 0.12 |
| (1,92) | 1:18:A:VAL:HG23 | 1:23:A:VAL:H | 20 | 0.12 |
| (1,69) | 1:16:A:SER:HB2 | 1:52:A:ASP:H | 15 | 0.12 |
| (1,69) | 1:16:A:SER:HB3 | 1:52:A:ASP:H | 15 | 0.12 |
| (1,64) | 1:15:A:GLU:HG2 | 2:123:B:SER:HA | 8 | 0.12 |
| (1,64) | 1:15:A:GLU:HG3 | 2:123:B:SER:HA | 8 | 0.12 |
| (1,57) | 1:15:A:GLU:H | 1:18:A:VAL:HG11 | 11 | 0.12 |
| (1,57) | 1:15:A:GLU:H | 1:18:A:VAL:HG12 | 11 | 0.12 |
| (1,57) | 1:15:A:GLU:H | 1:18:A:VAL:HG13 | 11 | 0.12 |
| (1,57) | 1:15:A:GLU:H | 1:18:A:VAL:HG21 | 11 | 0.12 |
| (1,57) | 1:15:A:GLU:H | 1:18:A:VAL:HG22 | 11 | 0.12 |
| (1,57) | 1:15:A:GLU:H | 1:18:A:VAL:HG23 | 11 | 0.12 |
| (1,43) | 1:14:A:PHE:H | 2:119:B:GLY:HA2 | 19 | 0.12 |
| (1,43) | 1:14:A:PHE:H | 2:119:B:GLY:HA3 | 19 | 0.12 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 19 | 0.11 |
| (3,37) | 1:240:C:ALA:O | 1:249:C:VAL:H | 6 | 0.11 |
| (3,28) | 1:224:C:LYS:N | 1:241:C:ARG:O | 10 | 0.11 |
| (3,23) | 1:40:A:ALA:O | 1:49:A:VAL:N | 18 | 0.11 |
| (3,22) | 1:40:A:ALA:O | 1:49:A:VAL:H | 20 | 0.11 |
| (3,16) | 1:28:A:ILE:O | 1:226:C:LEU:N | 18 | 0.11 |
| (3,15) | 1:28:A:ILE:O | 1:226:C:LEU:H | 7 | 0.11 |
| (3,9) | 1:27:A:LYS:H | 1:39:A:VAL:O | 4 | 0.11 |
| (3,8) | 1:26:A:LEU:O | 1:228:C:ILE:N | 10 | 0.11 |
| (3,5) | 1:26:A:LEU:H | 1:228:C:ILE:O | 18 | 0.11 |
| (3,3) | 1:24:A:LYS:H | 1:41:A:ARG:O | 11 | 0.11 |
| (3,2) | 1:11:A:CYS:SG | 1:50:A:CYS:SG | 19 | 0.11 |
| (2,17) | 1:211:C:CYS:CB | 1:250:C:CYS:SG | 3 | 0.11 |
| (2,17) | 1:211:C:CYS:CB | 1:250:C:CYS:SG | 17 | 0.11 |
| (2,14) | 1:209:C:CYS:CB | 1:234:C:CYS:SG | 17 | 0.11 |
| (2,13) | 1:209:C:CYS:CB | 1:234:C:CYS:CB | 12 | 0.11 |
| (2,6) | 1:11:A:CYS:SG | 1:50:A:CYS:CB | 6 | 0.11 |
| (2,6) | 1:11:A:CYS:SG | 1:50:A:CYS:CB | 19 | 0.11 |
| (2,5) | 1:11:A:CYS:CB | 1:50:A:CYS:SG | 1 | 0.11 |
| (2,5) | 1:11:A:CYS:CB | 1:50:A:CYS:SG | 5 | 0.11 |
| (2,5) | 1:11:A:CYS:CB | 1:50:A:CYS:SG | 19 | 0.11 |
| (2,2) | 1:9:A:CYS:CB | 1:34:A:CYS:SG | 2 | 0.11 |
| (2,2) | 1:9:A:CYS:CB | 1:34:A:CYS:SG | 11 | 0.11 |
| (2,2) | 1:9:A:CYS:CB | 1:34:A:CYS:SG | 16 | 0.11 |
| (2,2) | 1:9:A:CYS:CB | 1:34:A:CYS:SG | 17 | 0.11 |
| (2,1) | 1:9:A:CYS:CB | 1:34:A:CYS:CB | 5 | 0.11 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 7 | 0.11 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 11 | 0.11 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 11 | 0.11 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 15 | 0.11 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 15 | 0.11 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 16 | 0.11 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 16 | 0.11 |
| (1,1603) | 2:330:D:ARG:H | 2:330:D:ARG:HG2 | 12 | 0.11 |
| (1,1603) | 2:330:D:ARG:H | 2:330:D:ARG:HG3 | 12 | 0.11 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 3 | 0.11 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 3 | 0.11 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE1 | 17 | 0.11 |
| (1,1599) | 2:329:D:PHE:HA | 2:329:D:PHE:HE2 | 17 | 0.11 |
| (1,1594) | 2:328:D:ALA:HA | 2:329:D:PHE:H | 20 | 0.11 |
| (1,1591) | 2:327:D:PRO:HD2 | 2:328:D:ALA:H | 13 | 0.11 |
| (1,1591) | 2:327:D:PRO:HD3 | 2:328:D:ALA:H | 13 | 0.11 |
| (1,1587) | 2:325:D:LYS:HG2 | 2:326:D:GLU:H | 12 | 0.11 |
| (1,1587) | 2:325:D:LYS:HG3 | 2:326:D:GLU:H | 12 | 0.11 |
| (1,1578) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE2 | 13 | 0.11 |
| (1,1578) | 2:325:D:LYS:HB2 | 2:325:D:LYS:HE3 | 13 | 0.11 |
| (1,1573) | 2:325:D:LYS:H | 2:325:D:LYS:HG2 | 14 | 0.11 |
| (1,1573) | 2:325:D:LYS:H | 2:325:D:LYS:HG3 | 14 | 0.11 |
| (1,1533) | 2:313:D:THR:HA | 2:314:D:GLU:H | 3 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 5 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 5 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 5 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 6 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 6 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 6 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 7 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 7 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 7 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 8 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 8 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 8 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 13 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 13 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 13 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 15 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 15 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 15 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 19 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 19 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 19 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 20 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 20 | 0.11 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 20 | 0.11 |
| (1,1516) | 2:307:D:TYS:H | 2:307:D:TYS:HB3 | 6 | 0.11 |
| (1,1516) | 2:307:D:TYS:H | 2:307:D:TYS:HB3 | 6 | 0.11 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD2 | 4 | 0.11 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD3 | 4 | 0.11 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD2 | 13 | 0.11 |
| (1,1471) | 1:268:C:LYS:HA | 1:268:C:LYS:HD3 | 13 | 0.11 |
| (1,1470) | 1:268:C:LYS:H | 1:268:C:LYS:HG2 | 8 | 0.11 |
| (1,1470) | 1:268:C:LYS:H | 1:268:C:LYS:HG3 | 8 | 0.11 |
| (1,1465) | 1:267:C:ASN:HA | 1:268:C:LYS:H | 8 | 0.11 |
| (1,1443) | 1:264:C:LYS:HG2 | 1:265:C:CYS:H | 10 | 0.11 |
| (1,1439) | 1:264:C:LYS:HB3 | 1:264:C:LYS:HE2 | 5 | 0.11 |
| (1,1439) | 1:264:C:LYS:HB3 | 1:264:C:LYS:HE3 | 5 | 0.11 |
| (1,1433) | 1:264:C:LYS:HA | 1:264:C:LYS:HE2 | 16 | 0.11 |
| (1,1433) | 1:264:C:LYS:HA | 1:264:C:LYS:HE3 | 16 | 0.11 |
| (1,1430) | 1:264:C:LYS:H | 1:264:C:LYS:HE2 | 13 | 0.11 |
| (1,1430) | 1:264:C:LYS:H | 1:264:C:LYS:HE3 | 13 | 0.11 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 17 | 0.11 |
| (1,1306) | 1:255:C:LEU:H | 1:255:C:LEU:HG | 18 | 0.11 |
| (1,1289) | 1:254:C:LYS:H | 1:254:C:LYS:HE2 | 14 | 0.11 |
| (1,1289) | 1:254:C:LYS:H | 1:254:C:LYS:HE3 | 14 | 0.11 |
| (1,1244) | 1:251:C:ILE:H | 1:251:C:ILE:HD11 | 6 | 0.11 |
| (1,1244) | 1:251:C:ILE:H | 1:251:C:ILE:HD12 | 6 | 0.11 |
| (1,1244) | 1:251:C:ILE:H | 1:251:C:ILE:HD13 | 6 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 5 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 5 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 5 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 5 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 5 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 5 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 7 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 7 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 7 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 7 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 7 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 7 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 15 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 15 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 15 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 15 | 0.11 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 15 | 0.11 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 5 | 0.11 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 5 | 0.11 |
| (1,1157) | 1:238:C:ILE:HG21 | 1:251:C:ILE:HB | 20 | 0.11 |
| (1,1157) | 1:238:C:ILE:HG22 | 1:251:C:ILE:HB | 20 | 0.11 |
| (1,1157) | 1:238:C:ILE:HG23 | 1:251:C:ILE:HB | 20 | 0.11 |
| (1,1130) | 1:237:C:GLN:H | 1:253:C:PRO:HG3 | 4 | 0.11 |
| (1,1130) | 1:237:C:GLN:H | 1:253:C:PRO:HG3 | 11 | 0.11 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB2 | 18 | 0.11 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB3 | 18 | 0.11 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 1 | 0.11 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 1 | 0.11 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 11 | 0.11 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 11 | 0.11 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 17 | 0.11 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 17 | 0.11 |
| (1,1035) | 1:224:C:LYS:HG2 | 1:225:C:HIS:H | 3 | 0.11 |
| (1,1035) | 1:224:C:LYS:HG3 | 1:225:C:HIS:H | 3 | 0.11 |
| (1,1035) | 1:224:C:LYS:HG2 | 1:225:C:HIS:H | 4 | 0.11 |
| (1,1035) | 1:224:C:LYS:HG3 | 1:225:C:HIS:H | 4 | 0.11 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE1 | 1 | 0.11 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE2 | 1 | 0.11 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE1 | 1 | 0.11 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE2 | 1 | 0.11 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE1 | 6 | 0.11 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE2 | 6 | 0.11 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE1 | 6 | 0.11 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE2 | 6 | 0.11 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE1 | 11 | 0.11 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE2 | 11 | 0.11 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE1 | 11 | 0.11 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE2 | 11 | 0.11 |
| (1,961) | 1:218:C:VAL:HG11 | 1:252:C:ASP:H | 17 | 0.11 |
| (1,961) | 1:218:C:VAL:HG12 | 1:252:C:ASP:H | 17 | 0.11 |
| (1,961) | 1:218:C:VAL:HG13 | 1:252:C:ASP:H | 17 | 0.11 |
| (1,961) | 1:218:C:VAL:HG21 | 1:252:C:ASP:H | 17 | 0.11 |
| (1,961) | 1:218:C:VAL:HG22 | 1:252:C:ASP:H | 17 | 0.11 |
| (1,961) | 1:218:C:VAL:HG23 | 1:252:C:ASP:H | 17 | 0.11 |
| (1,952) | 1:218:C:VAL:HB | 1:255:C:LEU:HD11 | 20 | 0.11 |
| (1,952) | 1:218:C:VAL:HB | 1:255:C:LEU:HD12 | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,952) | 1:218:C:VAL:HB | 1:255:C:LEU:HD13 | 20 | 0.11 |
| (1,940) | 1:216:C:SER:HB2 | 1:252:C:ASP:H | 8 | 0.11 |
| (1,940) | 1:216:C:SER:HB3 | 1:252:C:ASP:H | 8 | 0.11 |
| (1,940) | 1:216:C:SER:HB2 | 1:252:C:ASP:H | 11 | 0.11 |
| (1,940) | 1:216:C:SER:HB3 | 1:252:C:ASP:H | 11 | 0.11 |
| (1,935) | 1:215:C:GLU:HG2 | 2:323:D:SER:HA | 8 | 0.11 |
| (1,935) | 1:215:C:GLU:HG3 | 2:323:D:SER:HA | 8 | 0.11 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD11 | 12 | 0.11 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD12 | 12 | 0.11 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD13 | 12 | 0.11 |
| (1,903) | 1:212:C:ARG:HD2 | 1:213:C:PHE:HE1 | 14 | 0.11 |
| (1,903) | 1:212:C:ARG:HD2 | 1:213:C:PHE:HE2 | 14 | 0.11 |
| (1,903) | 1:212:C:ARG:HD3 | 1:213:C:PHE:HE1 | 14 | 0.11 |
| (1,903) | 1:212:C:ARG:HD3 | 1:213:C:PHE:HE2 | 14 | 0.11 |
| (1,868) | 2:138:B:LYS:HA | 2:138:B:LYS:HE2 | 10 | 0.11 |
| (1,868) | 2:138:B:LYS:HA | 2:138:B:LYS:HE3 | 10 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 3 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 3 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 5 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 5 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 6 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 6 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 7 | 0.11 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 7 | 0.11 |
| (1,843) | 2:130:B:ARG:H | 2:130:B:ARG:HG2 | 6 | 0.11 |
| (1,843) | 2:130:B:ARG:H | 2:130:B:ARG:HG3 | 6 | 0.11 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE1 | 19 | 0.11 |
| (1,838) | 2:129:B:PHE:HA | 2:129:B:PHE:HE2 | 19 | 0.11 |
| (1,833) | 2:128:B:ALA:HA | 2:129:B:PHE:H | 2 | 0.11 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 17 | 0.11 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 17 | 0.11 |
| (1,828) | 2:127:B:PRO:HD2 | 2:128:B:ALA:H | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,828) | 2:127:B:PRO:HD3 | 2:128:B:ALA:H | 5 | 0.11 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD11 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD12 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD13 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD21 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD22 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB2 | 1:266:C:LEU:HD23 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD11 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD12 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD13 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD21 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD22 | 20 | 0.11 |
| (1,827) | 2:127:B:PRO:HB3 | 1:266:C:LEU:HD23 | 20 | 0.11 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE2 | 20 | 0.11 |
| (1,819) | 2:125:B:LYS:HB2 | 2:125:B:LYS:HE3 | 20 | 0.11 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE2 | 20 | 0.11 |
| (1,819) | 2:125:B:LYS:HB3 | 2:125:B:LYS:HE3 | 20 | 0.11 |
| (1,810) | 2:125:B:LYS:HA | 2:125:B:LYS:HD2 | 12 | 0.11 |
| (1,810) | 2:125:B:LYS:HA | 2:125:B:LYS:HD3 | 12 | 0.11 |
| (1,799) | 2:121:B:TYS:HA | 2:121:B:TYS:HD1 | 5 | 0.11 |
| (1,799) | 2:121:B:TYS:HA | 2:121:B:TYS:HD2 | 5 | 0.11 |
| (1,779) | 2:115:B:GLU:HA | 2:115:B:GLU:HG2 | 1 | 0.11 |
| (1,779) | 2:115:B:GLU:HA | 2:115:B:GLU:HG3 | 1 | 0.11 |
| (1,779) | 2:115:B:GLU:HA | 2:115:B:GLU:HG2 | 2 | 0.11 |
| (1,779) | 2:115:B:GLU:HA | 2:115:B:GLU:HG3 | 2 | 0.11 |
| (1,779) | 2:115:B:GLU:HA | 2:115:B:GLU:HG2 | 8 | 0.11 |
| (1,779) | 2:115:B:GLU:HA | 2:115:B:GLU:HG3 | 8 | 0.11 |
| (1,773) | 2:114:B:GLU:H | 2:114:B:GLU:HG2 | 5 | 0.11 |
| (1,773) | 2:114:B:GLU:H | 2:114:B:GLU:HG3 | 5 | 0.11 |
| (1,773) | 2:114:B:GLU:H | 2:114:B:GLU:HG2 | 9 | 0.11 |
| (1,773) | 2:114:B:GLU:H | 2:114:B:GLU:HG3 | 9 | 0.11 |
| (1,773) | 2:114:B:GLU:H | 2:114:B:GLU:HG2 | 11 | 0.11 |
| (1,773) | 2:114:B:GLU:H | 2:114:B:GLU:HG3 | 11 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 1 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 1 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 1 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 5 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 5 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 5 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 6 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 6 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 7 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 7 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 7 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 11 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 11 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 11 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 12 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 12 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 12 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 15 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 15 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 15 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 17 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 17 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 17 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 20 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 20 | 0.11 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 20 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 10 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 18 | 0.11 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE1 | 9 | 0.11 |
| (1,749) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HE2 | 9 | 0.11 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE1 | 9 | 0.11 |
| (1,749) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HE2 | 9 | 0.11 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE1 | 9 | 0.11 |
| (1,749) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HE2 | 9 | 0.11 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD1 | 4 | 0.11 |
| (1,748) | 2:106:B:ILE:HG21 | 2:107:B:TYS:HD2 | 4 | 0.11 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD1 | 4 | 0.11 |
| (1,748) | 2:106:B:ILE:HG22 | 2:107:B:TYS:HD2 | 4 | 0.11 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD1 | 4 | 0.11 |
| (1,748) | 2:106:B:ILE:HG23 | 2:107:B:TYS:HD2 | 4 | 0.11 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 4 | 0.11 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 4 | 0.11 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 5 | 0.11 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 17 | 0.11 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD2 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD11 | 2:327:D:PRO:HD3 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD2 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD12 | 2:327:D:PRO:HD3 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD2 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD13 | 2:327:D:PRO:HD3 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD2 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD21 | 2:327:D:PRO:HD3 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD2 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD22 | 2:327:D:PRO:HD3 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD2 | 18 | 0.11 |
| (1,692) | 1:66:A:LEU:HD23 | 2:327:D:PRO:HD3 | 18 | 0.11 |
| (1,652) | 1:64:A:LYS:HG2 | 1:65:A:CYS:H | 10 | 0.11 |
| (1,648) | 1:64:A:LYS:HB3 | 1:64:A:LYS:HE2 | 5 | 0.11 |
| (1,648) | 1:64:A:LYS:HB3 | 1:64:A:LYS:HE3 | 5 | 0.11 |
| (1,518) | 1:55:A:LEU:HD21 | 1:57:A:TRP:HZ2 | 7 | 0.11 |
| (1,518) | 1:55:A:LEU:HD22 | 1:57:A:TRP:HZ2 | 7 | 0.11 |
| (1,518) | 1:55:A:LEU:HD23 | 1:57:A:TRP:HZ2 | 7 | 0.11 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 8 | 0.11 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 11 | 0.11 |
| (1,490) | 1:55:A:LEU:H | 1:55:A:LEU:HG | 17 | 0.11 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 2 | 0.11 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 2 | 0.11 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 2 | 0.11 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 2 | 0.11 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 2 | 0.11 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 2 | 0.11 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 5 | 0.11 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 5 | 0.11 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 5 | 0.11 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 5 | 0.11 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 5 | 0.11 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 5 | 0.11 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 8 | 0.11 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 8 | 0.11 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 8 | 0.11 |
| (1,423) | 1:49:A:VAL:HG21 | 2:121:B:TYS:HB3 | 8 | 0.11 |
| (1,423) | 1:49:A:VAL:HG22 | 2:121:B:TYS:HB3 | 8 | 0.11 |
| (1,423) | 1:49:A:VAL:HG23 | 2:121:B:TYS:HB3 | 8 | 0.11 |
| (1,421) | 1:49:A:VAL:HG11 | 2:121:B:TYS:HE1 | 4 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG11 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG12 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG13 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG21 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG22 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG23 | 14 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG11 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG12 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG13 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG21 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG22 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG23 | 14 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG11 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG12 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG13 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG21 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG22 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE21 | 1:39:A:VAL:HG23 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG11 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG12 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG13 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG21 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG22 | 16 | 0.11 |
| (1,317) | 1:37:A:GLN:HE22 | 1:39:A:VAL:HG23 | 16 | 0.11 |
| (1,291) | 1:29:A:LEU:HD11 | 1:225:C:HIS:HE1 | 12 | 0.11 |
| (1,291) | 1:29:A:LEU:HD12 | 1:225:C:HIS:HE1 | 12 | 0.11 |
| (1,291) | 1:29:A:LEU:HD13 | 1:225:C:HIS:HE1 | 12 | 0.11 |
| (1,291) | 1:29:A:LEU:HD11 | 1:225:C:HIS:HE1 | 14 | 0.11 |
| (1,291) | 1:29:A:LEU:HD12 | 1:225:C:HIS:HE1 | 14 | 0.11 |
| (1,291) | 1:29:A:LEU:HD13 | 1:225:C:HIS:HE1 | 14 | 0.11 |
| (1,248) | 1:27:A:LYS:HE2 | 1:225:C:HIS:HE1 | 11 | 0.11 |
| (1,248) | 1:27:A:LYS:HE3 | 1:225:C:HIS:HE1 | 11 | 0.11 |
| (1,248) | 1:27:A:LYS:HE2 | 1:225:C:HIS:HE1 | 16 | 0.11 |
| (1,248) | 1:27:A:LYS:HE3 | 1:225:C:HIS:HE1 | 16 | 0.11 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE1 | 5 | 0.11 |
| (1,246) | 1:27:A:LYS:HE2 | 2:112:B:TYS:HE2 | 5 | 0.11 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE1 | 5 | 0.11 |
| (1,246) | 1:27:A:LYS:HE3 | 2:112:B:TYS:HE2 | 5 | 0.11 |
| (1,234) | 1:27:A:LYS:HD2 | 1:225:C:HIS:HE1 | 14 | 0.11 |
| (1,223) | 1:26:A:LEU:HD11 | 1:62:A:LEU:H | 6 | 0.11 |
| (1,223) | 1:26:A:LEU:HD12 | 1:62:A:LEU:H | 6 | 0.11 |
| (1,223) | 1:26:A:LEU:HD13 | 1:62:A:LEU:H | 6 | 0.11 |
| (1,223) | 1:26:A:LEU:HD21 | 1:62:A:LEU:H | 6 | 0.11 |
| (1,223) | 1:26:A:LEU:HD22 | 1:62:A:LEU:H | 6 | 0.11 |
| (1,223) | 1:26:A:LEU:HD23 | 1:62:A:LEU:H | 6 | 0.11 |
| (1,182) | 1:25:A:HIS:HE1 | 1:227:C:LYS:HE2 | 13 | 0.11 |
| (1,182) | 1:25:A:HIS:HE1 | 1:227:C:LYS:HE3 | 13 | 0.11 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 2 | 0.11 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 13 | 0.11 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG11 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG12 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG13 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG21 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG22 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,138) | 1:23:A:VAL:HG23 | 2:307:D:TYS:HB3 | 16 | 0.11 |
| (1,136) | 1:23:A:VAL:HB | 1:42:A:LEU:H | 20 | 0.11 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE1 | 2 | 0.11 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE2 | 2 | 0.11 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE1 | 2 | 0.11 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE2 | 2 | 0.11 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE1 | 16 | 0.11 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE2 | 16 | 0.11 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE1 | 16 | 0.11 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE2 | 16 | 0.11 |
| (1,92) | 1:18:A:VAL:HG11 | 1:23:A:VAL:H | 4 | 0.11 |
| (1,92) | 1:18:A:VAL:HG12 | 1:23:A:VAL:H | 4 | 0.11 |
| (1,92) | 1:18:A:VAL:HG13 | 1:23:A:VAL:H | 4 | 0.11 |
| (1,92) | 1:18:A:VAL:HG21 | 1:23:A:VAL:H | 4 | 0.11 |
| (1,92) | 1:18:A:VAL:HG22 | 1:23:A:VAL:H | 4 | 0.11 |
| (1,92) | 1:18:A:VAL:HG23 | 1:23:A:VAL:H | 4 | 0.11 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE1 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG11 | 2:121:B:TYS:HE2 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE1 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG12 | 2:121:B:TYS:HE2 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE1 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG13 | 2:121:B:TYS:HE2 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE1 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG21 | 2:121:B:TYS:HE2 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE1 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG22 | 2:121:B:TYS:HE2 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE1 | 18 | 0.11 |
| (1,87) | 1:18:A:VAL:HG23 | 2:121:B:TYS:HE2 | 18 | 0.11 |
| (1,69) | 1:16:A:SER:HB2 | 1:52:A:ASP:H | 20 | 0.11 |
| (1,69) | 1:16:A:SER:HB3 | 1:52:A:ASP:H | 20 | 0.11 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD11 | 6 | 0.11 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD12 | 6 | 0.11 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD13 | 6 | 0.11 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD11 | 17 | 0.11 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD12 | 17 | 0.11 |
| (1,59) | 1:15:A:GLU:H | 1:51:A:ILE:HD13 | 17 | 0.11 |
| (1,12) | 1:10:A:PRO:HB2 | 2:112:B:TYS:HE1 | 11 | 0.11 |
| (3,38) | 1:240:C:ALA:O | 1:249:C:VAL:N | 14 | 0.1 |
| (3,20) | 1:40:A:ALA:H | 1:49:A:VAL:O | 10 | 0.1 |
| (3,16) | 1:28:A:ILE:O | 1:226:C:LEU:N | 15 | 0.1 |
| (2,18) | 1:211:C:CYS:SG | 1:250:C:CYS:CB | 5 | 0.1 |
| (2,18) | 1:211:C:CYS:SG | 1:250:C:CYS:CB | 9 | 0.1 |
| (2,18) | 1:211:C:CYS:SG | 1:250:C:CYS:CB | 18 | 0.1 |
| (2,17) | 1:211:C:CYS:CB | 1:250:C:CYS:SG | 5 | 0.1 |
| (2,17) | 1:211:C:CYS:CB | 1:250:C:CYS:SG | 6 | 0.1 |
| (2,7) | 1:36:A:CYS:CB | 1:265:C:CYS:CB | 15 | 0.1 |
| (2,6) | 1:11:A:CYS:SG | 1:50:A:CYS:CB | 17 | 0.1 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE1 | 1 | 0.1 |
| (1,1626) | 2:336:D:PHE:HA | 2:336:D:PHE:HE2 | 1 | 0.1 |
| (1,1623) | 2:332:D:GLU:HA | 2:332:D:GLU:HG2 | 14 | 0.1 |
| (1,1623) | 2:332:D:GLU:HA | 2:332:D:GLU:HG3 | 14 | 0.1 |
| (1,1623) | 2:332:D:GLU:HA | 2:332:D:GLU:HG2 | 16 | 0.1 |
| (1,1623) | 2:332:D:GLU:HA | 2:332:D:GLU:HG3 | 16 | 0.1 |
| (1,1622) | 2:332:D:GLU:H | 2:332:D:GLU:HG2 | 7 | 0.1 |
| (1,1622) | 2:332:D:GLU:H | 2:332:D:GLU:HG3 | 7 | 0.1 |
| (1,1592) | 2:327:D:PRO:HG2 | 2:328:D:ALA:H | 8 | 0.1 |
| (1,1592) | 2:327:D:PRO:HG3 | 2:328:D:ALA:H | 8 | 0.1 |
| (1,1592) | 2:327:D:PRO:HG2 | 2:328:D:ALA:H | 10 | 0.1 |
| (1,1592) | 2:327:D:PRO:HG3 | 2:328:D:ALA:H | 10 | 0.1 |
| (1,1543) | 2:315:D:GLU:HA | 2:315:D:GLU:HG2 | 18 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,1543) | 2:315:D:GLU:HA | 2:315:D:GLU:HG3 | 18 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 1 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 1 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 1 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 2 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 2 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 2 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG21 | 9 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG22 | 9 | 0.1 |
| (1,1532) | 2:313:D:THR:HA | 2:313:D:THR:HG23 | 9 | 0.1 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 20 | 0.1 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 20 | 0.1 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 20 | 0.1 |
| (1,1240) | 1:249:C:VAL:HG21 | 2:321:D:TYS:HB3 | 20 | 0.1 |
| (1,1240) | 1:249:C:VAL:HG22 | 2:321:D:TYS:HB3 | 20 | 0.1 |
| (1,1240) | 1:249:C:VAL:HG23 | 2:321:D:TYS:HB3 | 20 | 0.1 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD2 | 11 | 0.1 |
| (1,1222) | 1:247:C:ARG:HA | 1:247:C:ARG:HD3 | 11 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG11 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG12 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG13 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG21 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG22 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE21 | 1:239:C:VAL:HG23 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG11 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG12 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG13 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG21 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG22 | 10 | 0.1 |
| (1,1133) | 1:237:C:GLN:HE22 | 1:239:C:VAL:HG23 | 10 | 0.1 |
| (1,1130) | 1:237:C:GLN:H | 1:253:C:PRO:HG3 | 20 | 0.1 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB2 | 14 | 0.1 |
| (1,1043) | 1:225:C:HIS:HE1 | 1:241:C:ARG:HB3 | 14 | 0.1 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 3 | 0.1 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 3 | 0.1 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE2 | 18 | 0.1 |
| (1,1042) | 1:225:C:HIS:HE1 | 1:227:C:LYS:HE3 | 18 | 0.1 |
| (1,1032) | 1:224:C:LYS:HE2 | 1:241:C:ARG:H | 5 | 0.1 |
| (1,1032) | 1:224:C:LYS:HE3 | 1:241:C:ARG:H | 5 | 0.1 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE1 | 2 | 0.1 |
| (1,986) | 1:220:C:ARG:HD2 | 1:261:C:TYR:HE2 | 2 | 0.1 |
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE1 | 2 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,986) | 1:220:C:ARG:HD3 | 1:261:C:TYR:HE2 | 2 | 0.1 |
| (1,960) | 1:218:C:VAL:HG11 | 1:223:C:VAL:H | 1 | 0.1 |
| (1,960) | 1:218:C:VAL:HG12 | 1:223:C:VAL:H | 1 | 0.1 |
| (1,960) | 1:218:C:VAL:HG13 | 1:223:C:VAL:H | 1 | 0.1 |
| (1,960) | 1:218:C:VAL:HG21 | 1:223:C:VAL:H | 1 | 0.1 |
| (1,960) | 1:218:C:VAL:HG22 | 1:223:C:VAL:H | 1 | 0.1 |
| (1,960) | 1:218:C:VAL:HG23 | 1:223:C:VAL:H | 1 | 0.1 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD11 | 6 | 0.1 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD12 | 6 | 0.1 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD13 | 6 | 0.1 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD11 | 8 | 0.1 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD12 | 8 | 0.1 |
| (1,930) | 1:215:C:GLU:H | 1:251:C:ILE:HD13 | 8 | 0.1 |
| (1,868) | 2:138:B:LYS:HA | 2:138:B:LYS:HE2 | 20 | 0.1 |
| (1,868) | 2:138:B:LYS:HA | 2:138:B:LYS:HE3 | 20 | 0.1 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 12 | 0.1 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 12 | 0.1 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE1 | 17 | 0.1 |
| (1,866) | 2:136:B:PHE:HA | 2:136:B:PHE:HE2 | 17 | 0.1 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG2 | 8 | 0.1 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG3 | 8 | 0.1 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG2 | 14 | 0.1 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG3 | 14 | 0.1 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG2 | 19 | 0.1 |
| (1,863) | 2:132:B:GLU:HA | 2:132:B:GLU:HG3 | 19 | 0.1 |
| (1,846) | 2:130:B:ARG:HA | 2:131:B:GLU:H | 6 | 0.1 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD11 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD12 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD13 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD21 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD22 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD2 | 1:266:C:LEU:HD23 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD11 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD12 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD13 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD21 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD22 | 10 | 0.1 |
| (1,829) | 2:127:B:PRO:HD3 | 1:266:C:LEU:HD23 | 10 | 0.1 |
| (1,828) | 2:127:B:PRO:HD2 | 2:128:B:ALA:H | 3 | 0.1 |
| (1,828) | 2:127:B:PRO:HD3 | 2:128:B:ALA:H | 3 | 0.1 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB2 | 5 | 0.1 |
| (1,801) | 2:121:B:TYS:HD1 | 2:122:B:ASP:HB3 | 5 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB2 | 5 | 0.1 |
| (1,801) | 2:121:B:TYS:HD2 | 2:122:B:ASP:HB3 | 5 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 8 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 8 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 8 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 9 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 9 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 9 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG21 | 18 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG22 | 18 | 0.1 |
| (1,768) | 2:113:B:THR:HA | 2:113:B:THR:HG23 | 18 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG11 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG12 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG13 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG21 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG22 | 4 | 0.1 |
| (1,753) | 2:107:B:TYS:HB3 | 1:223:C:VAL:HG23 | 4 | 0.1 |
| (1,744) | 2:106:B:ILE:HG12 | 2:107:B:TYS:H | 1 | 0.1 |
| (1,744) | 2:106:B:ILE:HG13 | 2:107:B:TYS:H | 1 | 0.1 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 12 | 0.1 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 12 | 0.1 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD2 | 19 | 0.1 |
| (1,705) | 1:68:A:LYS:HA | 1:68:A:LYS:HD3 | 19 | 0.1 |
| (1,699) | 1:67:A:ASN:HA | 1:68:A:LYS:H | 9 | 0.1 |
| (1,531) | 1:56:A:LYS:HD2 | 1:60:A:GLU:HG2 | 17 | 0.1 |
| (1,531) | 1:56:A:LYS:HD3 | 1:60:A:GLU:HG2 | 17 | 0.1 |
| (1,473) | 1:54:A:LYS:H | 1:54:A:LYS:HE2 | 14 | 0.1 |
| (1,473) | 1:54:A:LYS:H | 1:54:A:LYS:HE3 | 14 | 0.1 |
| (1,248) | 1:27:A:LYS:HE2 | 1:225:C:HIS:HE1 | 8 | 0.1 |
| (1,248) | 1:27:A:LYS:HE3 | 1:225:C:HIS:HE1 | 8 | 0.1 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 8 | 0.1 |
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 8 | 0.1 |
| (1,166) | 1:24:A:LYS:HG2 | 1:25:A:HIS:H | 17 | 0.1 |
| (1,166) | 1:24:A:LYS:HG3 | 1:25:A:HIS:H | 17 | 0.1 |
| (1,145) | 1:24:A:LYS:H | 1:24:A:LYS:HD2 | 18 | 0.1 |
| (1,145) | 1:24:A:LYS:H | 1:24:A:LYS:HD3 | 18 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE1 | 3 | 0.1 |
| (1,115) | 1:20:A:ARG:HD2 | 1:61:A:TYR:HE2 | 3 | 0.1 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE1 | 3 | 0.1 |
| (1,115) | 1:20:A:ARG:HD3 | 1:61:A:TYR:HE2 | 3 | 0.1 |
| (1,112) | 1:20:A:ARG:HB2 | 1:57:A:TRP:HH2 | 18 | 0.1 |
| (1,112) | 1:20:A:ARG:HB3 | 1:57:A:TRP:HH2 | 18 | 0.1 |
| (1,98) | 1:19:A:ALA:H | 1:22:A:ASN:HD21 | 11 | 0.1 |
| (1,98) | 1:19:A:ALA:H | 1:22:A:ASN:HD22 | 11 | 0.1 |

# 10 Dihedral-angle violation analysis (i)

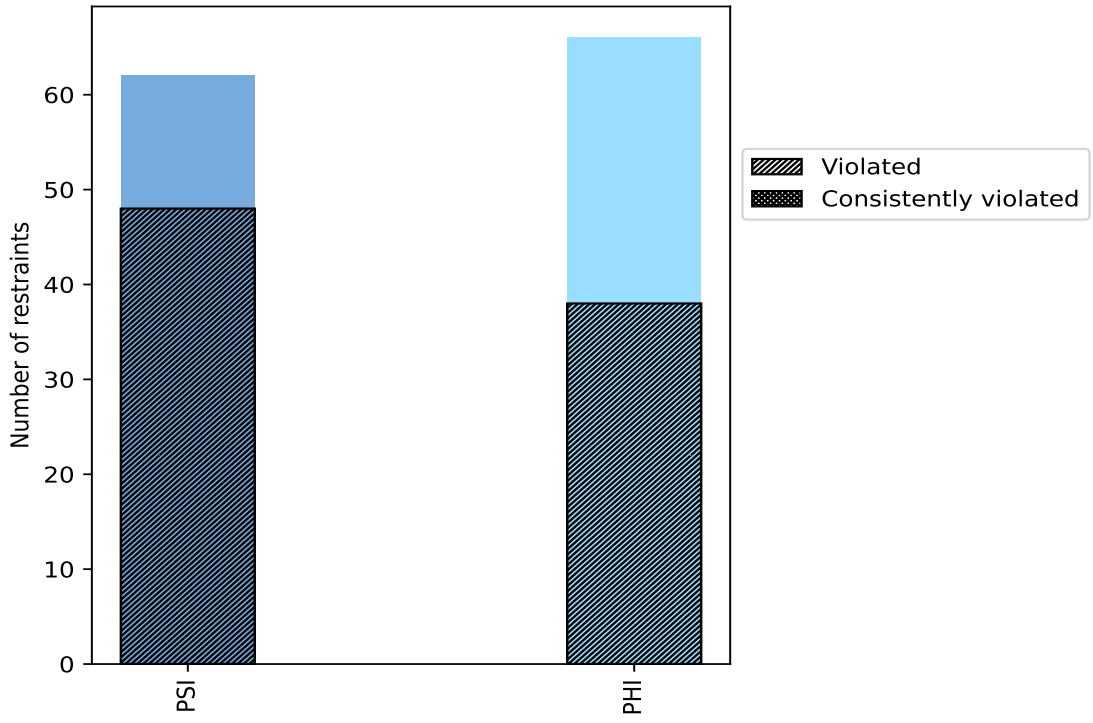
## 10.1 Summary of dihedral-angle violations (i)

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

| Angle type | Count | %[1] | Violated[3] | | | Consistently Violated[4] | | |
|---|---|---|---|---|---|---|---|---|
| | | | Count | %[2] | %[1] | Count | %[2] | %[1] |
| PSI | 62 | 48.4 | 48 | 77.4 | 37.5 | 0 | 0.0 | 0.0 |
| PHI | 66 | 51.6 | 38 | 57.6 | 29.7 | 0 | 0.0 | 0.0 |
| Total | 128 | 100.0 | 86 | 67.2 | 67.2 | 0 | 0.0 | 0.0 |

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

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



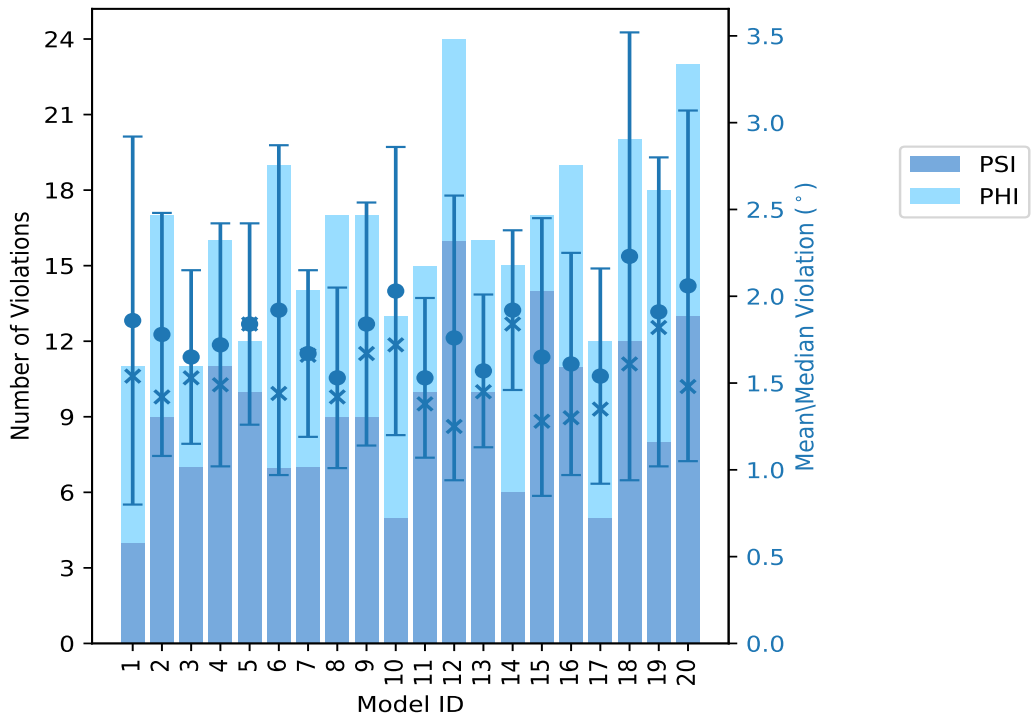

Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|---|---|---|---|---|---|---|---|
| | PSI | PHI | Total | | | | |
| 1 | 4 | 7 | 11 | 1.86 | 4.85 | 1.06 | 1.54 |
| 2 | 9 | 8 | 17 | 1.78 | 3.12 | 0.7 | 1.42 |
| 3 | 7 | 4 | 11 | 1.65 | 2.66 | 0.5 | 1.53 |
| 4 | 11 | 5 | 16 | 1.72 | 3.52 | 0.7 | 1.49 |
| 5 | 10 | 2 | 12 | 1.84 | 3.3 | 0.58 | 1.84 |
| 6 | 7 | 12 | 19 | 1.92 | 4.54 | 0.95 | 1.44 |
| 7 | 7 | 7 | 14 | 1.67 | 2.63 | 0.48 | 1.66 |
| 8 | 9 | 8 | 17 | 1.53 | 2.74 | 0.52 | 1.42 |
| 9 | 9 | 8 | 17 | 1.84 | 3.42 | 0.7 | 1.67 |
| 10 | 5 | 8 | 13 | 2.03 | 3.43 | 0.83 | 1.72 |
| 11 | 10 | 5 | 15 | 1.53 | 3.05 | 0.46 | 1.38 |
| 12 | 16 | 8 | 24 | 1.76 | 3.55 | 0.82 | 1.25 |
| 13 | 10 | 6 | 16 | 1.57 | 2.58 | 0.44 | 1.45 |
| 14 | 6 | 9 | 15 | 1.92 | 2.66 | 0.46 | 1.84 |
| 15 | 14 | 3 | 17 | 1.65 | 3.64 | 0.8 | 1.28 |
| 16 | 11 | 8 | 19 | 1.61 | 3.78 | 0.64 | 1.3 |
| 17 | 5 | 7 | 12 | 1.54 | 3.12 | 0.62 | 1.35 |
| 18 | 12 | 8 | 20 | 2.23 | 4.94 | 1.29 | 1.61 |
| 19 | 8 | 10 | 18 | 1.91 | 3.93 | 0.89 | 1.82 |
| 20 | 13 | 10 | 23 | 2.06 | 3.95 | 1.01 | 1.48 |

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




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

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

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

| Number of violated restraints | | | Fraction of the ensemble | |
|---|---|---|---|---|
| PSI | PHI | Total | Count[1] | % |
| 16 | 11 | 27 | 1 | 5.0 |
| 8 | 7 | 15 | 2 | 10.0 |
| 5 | 3 | 8 | 3 | 15.0 |
| 4 | 5 | 9 | 4 | 20.0 |
| 2 | 4 | 6 | 5 | 25.0 |
| 3 | 3 | 6 | 6 | 30.0 |
| 2 | 0 | 2 | 7 | 35.0 |
| 1 | 1 | 2 | 8 | 40.0 |
| 3 | 0 | 3 | 9 | 45.0 |
| 2 | 2 | 4 | 10 | 50.0 |
| 1 | 1 | 2 | 11 | 55.0 |

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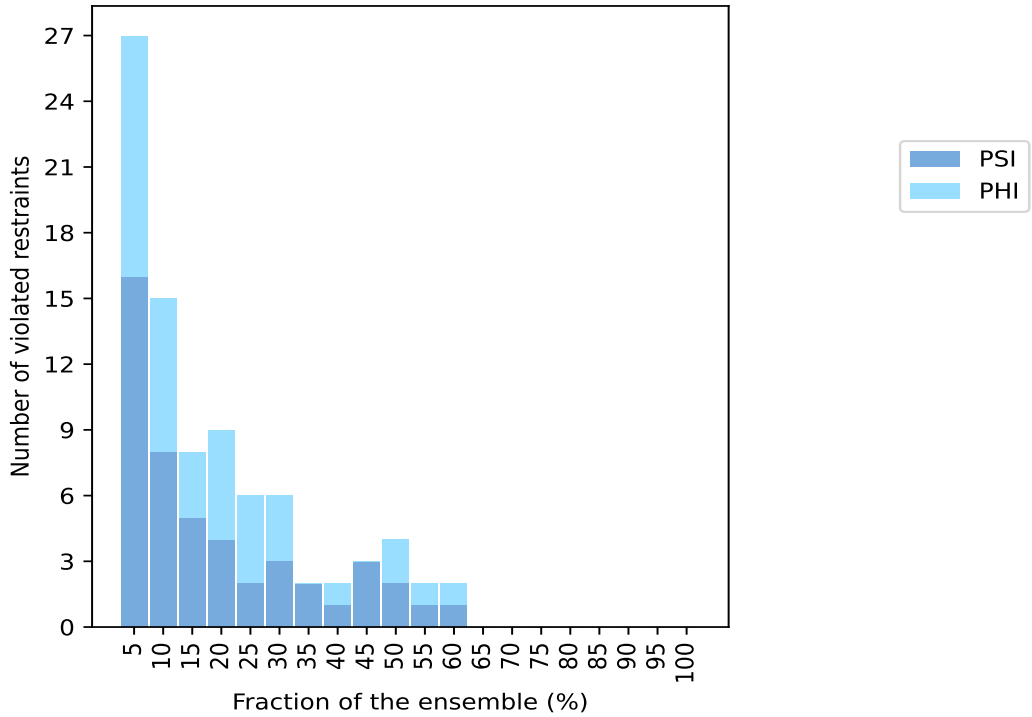
| Number of violated restraints | | | Fraction of the ensemble | |
|---|---|---|---|---|
| PSI | PHI | Total | Count[1] | % |
| 1 | 1 | 2 | 12 | 60.0 |
| 0 | 0 | 0 | 13 | 65.0 |
| 0 | 0 | 0 | 14 | 70.0 |
| 0 | 0 | 0 | 15 | 75.0 |
| 0 | 0 | 0 | 16 | 80.0 |
| 0 | 0 | 0 | 17 | 85.0 |
| 0 | 0 | 0 | 18 |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

[1] Number of models with violations

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

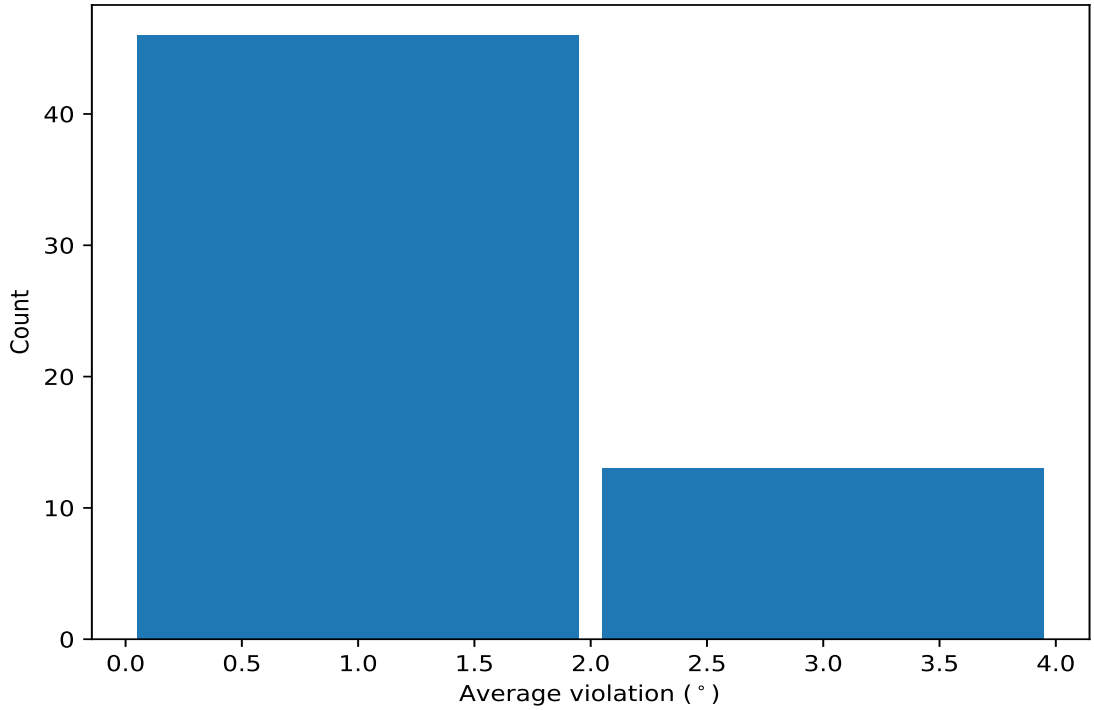



## 10.4 Most violated dihedral-angle restraints in the ensemble (i)

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

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

in the ensemble




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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models[1] | Mean | SD[2] | Median |
|---|---|---|---|---|---|---|---|---|
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 12 | 2.64 | 1.26 | 2.37 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 12 | 1.96 | 0.75 | 1.74 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 11 | 2.21 | 0.74 | 2.18 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 11 | 2.07 | 0.93 | 1.63 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 10 | 2.54 | 1.11 | 2.72 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 10 | 2.19 | 0.77 | 2.05 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 10 | 1.63 | 0.56 | 1.62 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 10 | 1.31 | 0.25 | 1.27 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 9 | 2.76 | 0.91 | 2.55 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 9 | 2.07 | 0.7 | 1.78 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 9 | 1.69 | 0.74 | 1.32 |
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 8 | 2.06 | 1.3 | 1.37 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 8 | 1.72 | 0.59 | 1.57 |
| (1,18) | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1:22:A:ASN:N | 7 | 1.52 | 0.5 | 1.32 |
| (1,114) | 1:257:C:TRP:N | 1:257:C:TRP:CA | 1:257:C:TRP:C | 1:258:C:ILE:N | 7 | 1.48 | 0.42 | 1.27 |
| (1,128) | 1:264:C:LYS:N | 1:264:C:LYS:CA | 1:264:C:LYS:C | 1:265:C:CYS:N | 6 | 2.23 | 1.11 | 2.06 |
| (1,19) | 1:22:A:ASN:C | 1:23:A:VAL:N | 1:23:A:VAL:CA | 1:23:A:VAL:C | 6 | 2.18 | 0.59 | 2.22 |
| (1,105) | 1:247:C:ARG:C | 1:248:C:GLN:N | 1:248:C:GLN:CA | 1:248:C:GLN:C | 6 | 1.9 | 0.7 | 1.62 |
| (1,82) | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 1:222:C:ASN:N | 6 | 1.67 | 0.4 | 1.71 |
| (1,95) | 1:233:C:ASN:C | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 6 | 1.46 | 0.28 | 1.44 |

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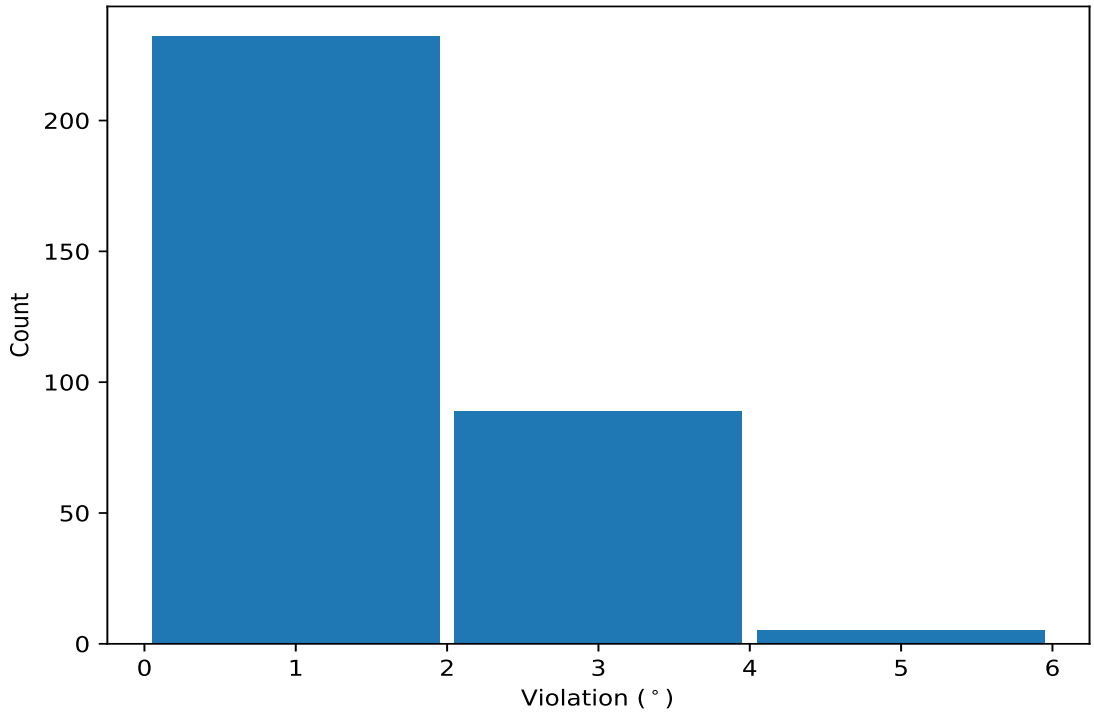
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models[1] | Mean | SD[2] | Median |
|---|---|---|---|---|---|---|---|---|
| (1,94) | 1:231:C:THR:N | 1:231:C:THR:CA | 1:231:C:THR:C | 1:232:C:PRO:N | 6 | 1.42 | 0.41 | 1.2 |
| (1,64) | 1:64:A:LYS:N | 1:64:A:LYS:CA | 1:64:A:LYS:C | 1:65:A:CYS:N | 5 | 2.92 | 0.6 | 3.05 |
| (1,73) | 1:213:C:PHE:C | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 5 | 1.61 | 0.65 | 1.29 |
| (1,3) | 1:8:A:ARG:C | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 5 | 1.58 | 0.6 | 1.31 |
| (1,54) | 1:59:A:GLN:N | 1:59:A:GLN:CA | 1:59:A:GLN:C | 1:60:A:GLU:N | 5 | 1.49 | 0.51 | 1.42 |
| (1,17) | 1:20:A:ARG:C | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 5 | 1.34 | 0.32 | 1.17 |
| (1,85) | 1:225:C:HIS:C | 1:226:C:LEU:N | 1:226:C:LEU:CA | 1:226:C:LEU:C | 5 | 1.18 | 0.07 | 1.21 |
| (1,21) | 1:25:A:HIS:C | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C | 4 | 1.66 | 0.55 | 1.63 |
| (1,91) | 1:229:C:LEU:C | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 4 | 1.64 | 0.53 | 1.6 |
| (1,66) | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 1:209:C:CYS:N | 4 | 1.61 | 0.77 | 1.25 |
| (1,31) | 1:33:A:ASN:C | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 4 | 1.55 | 0.33 | 1.48 |
| (1,2) | 1:8:A:ARG:N | 1:8:A:ARG:CA | 1:8:A:ARG:C | 1:9:A:CYS:N | 4 | 1.51 | 0.41 | 1.43 |
| (1,83) | 1:222:C:ASN:C | 1:223:C:VAL:N | 1:223:C:VAL:CA | 1:223:C:VAL:C | 4 | 1.4 | 0.18 | 1.33 |
| (1,89) | 1:227:C:LYS:C | 1:228:C:ILE:N | 1:228:C:ILE:CA | 1:228:C:ILE:C | 4 | 1.39 | 0.21 | 1.36 |
| (1,74) | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 1:215:C:GLU:N | 4 | 1.35 | 0.51 | 1.08 |
| (1,24) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:ILE:N | 4 | 1.27 | 0.22 | 1.28 |
| (1,9) | 1:13:A:PHE:C | 1:14:A:PHE:N | 1:14:A:PHE:CA | 1:14:A:PHE:C | 3 | 2.15 | 0.69 | 1.84 |
| (1,81) | 1:220:C:ARG:C | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 3 | 1.59 | 0.37 | 1.42 |
| (1,16) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:ALA:N | 3 | 1.58 | 0.59 | 1.28 |
| (1,56) | 1:60:A:GLU:N | 1:60:A:GLU:CA | 1:60:A:GLU:C | 1:61:A:TYR:N | 3 | 1.56 | 0.19 | 1.61 |
| (1,65) | 1:207:C:TYR:C | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 3 | 1.52 | 0.36 | 1.27 |
| (1,12) | 1:15:A:GLU:N | 1:15:A:GLU:CA | 1:15:A:GLU:C | 1:16:A:SER:N | 3 | 1.48 | 0.36 | 1.54 |
| (1,92) | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 1:231:C:THR:N | 3 | 1.39 | 0.35 | 1.23 |
| (1,40) | 1:41:A:ARG:N | 1:41:A:ARG:CA | 1:41:A:ARG:C | 1:42:A:LEU:N | 3 | 1.24 | 0.2 | 1.18 |
| (1,8) | 1:13:A:PHE:N | 1:13:A:PHE:CA | 1:13:A:PHE:C | 1:14:A:PHE:N | 2 | 2.78 | 0.12 | 2.78 |
| (1,80) | 1:220:C:ARG:N | 1:220:C:ARG:CA | 1:220:C:ARG:C | 1:221:C:ALA:N | 2 | 1.88 | 0.64 | 1.88 |
| (1,75) | 1:214:C:PHE:C | 1:215:C:GLU:N | 1:215:C:GLU:CA | 1:215:C:GLU:C | 2 | 1.86 | 0.02 | 1.86 |
| (1,39) | 1:40:A:ALA:C | 1:41:A:ARG:N | 1:41:A:ARG:CA | 1:41:A:ARG:C | 2 | 1.76 | 0.24 | 1.76 |
| (1,72) | 1:213:C:PHE:N | 1:213:C:PHE:CA | 1:213:C:PHE:C | 1:214:C:PHE:N | 2 | 1.76 | 0.46 | 1.76 |
| (1,28) | 1:30:A:ASN:N | 1:30:A:ASN:CA | 1:30:A:ASN:C | 1:31:A:THR:N | 2 | 1.68 | 0.57 | 1.68 |
| (1,29) | 1:30:A:ASN:C | 1:31:A:THR:N | 1:31:A:THR:CA | 1:31:A:THR:C | 2 | 1.6 | 0.34 | 1.6 |
| (1,1) | 1:7:A:TYR:C | 1:8:A:ARG:N | 1:8:A:ARG:CA | 1:8:A:ARG:C | 2 | 1.48 | 0.21 | 1.48 |
| (1,88) | 1:227:C:LYS:N | 1:227:C:LYS:CA | 1:227:C:LYS:C | 1:228:C:ILE:N | 2 | 1.44 | 0.07 | 1.44 |
| (1,120) | 1:260:C:GLU:N | 1:260:C:GLU:CA | 1:260:C:GLU:C | 1:261:C:TYR:N | 2 | 1.38 | 0.01 | 1.38 |
| (1,27) | 1:29:A:LEU:C | 1:30:A:ASN:N | 1:30:A:ASN:CA | 1:30:A:ASN:C | 2 | 1.16 | 0.05 | 1.16 |
| (1,15) | 1:19:A:ALA:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 2 | 1.12 | 0.04 | 1.12 |
| (1,103) | 1:240:C:ALA:C | 1:241:C:ARG:N | 1:241:C:ARG:CA | 1:241:C:ARG:C | 2 | 1.12 | 0.09 | 1.12 |
| (1,110) | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 1:251:C:ILE:N | 2 | 1.12 | 0.12 | 1.12 |
| (1,30) | 1:31:A:THR:N | 1:31:A:THR:CA | 1:31:A:THR:C | 1:32:A:PRO:N | 2 | 1.03 | 0.03 | 1.03 |

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

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

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

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




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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 18 | 4.94 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 1 | 4.85 |
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 18 | 4.78 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 6 | 4.54 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 18 | 4.1 |
| (1,78) | 1:219:C:ALA:N | 1:219:C:ALA:CA | 1:219:C:ALA:C | 1:220:C:ARG:N | 20 | 3.95 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 19 | 3.93 |
| (1,128) | 1:264:C:LYS:N | 1:264:C:LYS:CA | 1:264:C:LYS:C | 1:265:C:CYS:N | 20 | 3.83 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 18 | 3.83 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 16 | 3.78 |
| (1,64) | 1:64:A:LYS:N | 1:64:A:LYS:CA | 1:64:A:LYS:C | 1:65:A:CYS:N | 20 | 3.78 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 19 | 3.73 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 18 | 3.68 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 6 | 3.68 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 15 | 3.64 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 12 | 3.55 |
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 4 | 3.52 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 12 | 3.51 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 15 | 3.43 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 10 | 3.43 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 9 | 3.42 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,67) | 1:208:C:ARG:C | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 20 | 3.37 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 20 | 3.34 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 10 | 3.33 |
| (1,128) | 1:264:C:LYS:N | 1:264:C:LYS:CA | 1:264:C:LYS:C | 1:265:C:CYS:N | 5 | 3.3 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 10 | 3.27 |
| (1,64) | 1:64:A:LYS:N | 1:64:A:LYS:CA | 1:64:A:LYS:C | 1:65:A:CYS:N | 12 | 3.26 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 18 | 3.26 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 6 | 3.2 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 17 | 3.12 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 2 | 3.12 |
| (1,9) | 1:13:A:PHE:C | 1:14:A:PHE:N | 1:14:A:PHE:CA | 1:14:A:PHE:C | 19 | 3.1 |
| (1,64) | 1:64:A:LYS:N | 1:64:A:LYS:CA | 1:64:A:LYS:C | 1:65:A:CYS:N | 11 | 3.05 |
| (1,105) | 1:247:C:ARG:C | 1:248:C:GLN:N | 1:248:C:GLN:CA | 1:248:C:GLN:C | 2 | 3.03 |
| (1,19) | 1:22:A:ASN:C | 1:23:A:VAL:N | 1:23:A:VAL:CA | 1:23:A:VAL:C | 2 | 2.98 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 20 | 2.94 |
| (1,66) | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 1:209:C:CYS:N | 20 | 2.92 |
| (1,73) | 1:213:C:PHE:C | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 4 | 2.9 |
| (1,8) | 1:13:A:PHE:N | 1:13:A:PHE:CA | 1:13:A:PHE:C | 1:14:A:PHE:N | 9 | 2.9 |
| (1,128) | 1:264:C:LYS:N | 1:264:C:LYS:CA | 1:264:C:LYS:C | 1:265:C:CYS:N | 12 | 2.74 |
| (1,3) | 1:8:A:ARG:C | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 8 | 2.74 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 12 | 2.72 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 1 | 2.69 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 9 | 2.66 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 14 | 2.66 |
| (1,8) | 1:13:A:PHE:N | 1:13:A:PHE:CA | 1:13:A:PHE:C | 1:14:A:PHE:N | 3 | 2.66 |
| (1,19) | 1:22:A:ASN:C | 1:23:A:VAL:N | 1:23:A:VAL:CA | 1:23:A:VAL:C | 6 | 2.65 |
| (1,105) | 1:247:C:ARG:C | 1:248:C:GLN:N | 1:248:C:GLN:CA | 1:248:C:GLN:C | 14 | 2.64 |
| (1,18) | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1:22:A:ASN:N | 7 | 2.63 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 9 | 2.61 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 10 | 2.59 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 20 | 2.58 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 13 | 2.58 |
| (1,19) | 1:22:A:ASN:C | 1:23:A:VAL:N | 1:23:A:VAL:CA | 1:23:A:VAL:C | 8 | 2.56 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 19 | 2.55 |
| (1,80) | 1:220:C:ARG:N | 1:220:C:ARG:CA | 1:220:C:ARG:C | 1:221:C:ALA:N | 2 | 2.52 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 17 | 2.51 |
| (1,54) | 1:59:A:GLN:N | 1:59:A:GLN:CA | 1:59:A:GLN:C | 1:60:A:GLU:N | 14 | 2.46 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 14 | 2.43 |
| (1,16) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:ALA:N | 4 | 2.41 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 7 | 2.4 |
| (1,91) | 1:229:C:LEU:C | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 13 | 2.36 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 16 | 2.35 |
| (1,21) | 1:25:A:HIS:C | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C | 5 | 2.35 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 6 | 2.34 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 20 | 2.33 |
| (1,114) | 1:257:C:TRP:N | 1:257:C:TRP:CA | 1:257:C:TRP:C | 1:258:C:ILE:N | 7 | 2.32 |
| (1,64) | 1:64:A:LYS:N | 1:64:A:LYS:CA | 1:64:A:LYS:C | 1:65:A:CYS:N | 15 | 2.29 |
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 15 | 2.29 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 8 | 2.27 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 9 | 2.25 |
| (1,28) | 1:30:A:ASN:N | 1:30:A:ASN:CA | 1:30:A:ASN:C | 1:31:A:THR:N | 3 | 2.25 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,74) | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 1:215:C:GLU:N | 12 | 2.23 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 9 | 2.22 |
| (1,72) | 1:213:C:PHE:N | 1:213:C:PHE:CA | 1:213:C:PHE:C | 1:214:C:PHE:N | 4 | 2.22 |
| (1,64) | 1:64:A:LYS:N | 1:64:A:LYS:CA | 1:64:A:LYS:C | 1:65:A:CYS:N | 18 | 2.21 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 1 | 2.18 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 19 | 2.18 |
| (1,82) | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 1:222:C:ASN:N | 5 | 2.17 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 10 | 2.16 |
| (1,2) | 1:8:A:ARG:N | 1:8:A:ARG:CA | 1:8:A:ARG:C | 1:9:A:CYS:N | 2 | 2.16 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 3 | 2.11 |
| (1,81) | 1:220:C:ARG:C | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 14 | 2.1 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 19 | 2.1 |
| (1,98) | 1:238:C:ILE:N | 1:238:C:ILE:CA | 1:238:C:ILE:C | 1:239:C:VAL:N | 12 | 2.07 |
| (1,82) | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 1:222:C:ASN:N | 16 | 2.06 |
| (1,31) | 1:33:A:ASN:C | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 14 | 2.06 |
| (1,21) | 1:25:A:HIS:C | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C | 6 | 2.05 |
| (1,94) | 1:231:C:THR:N | 1:231:C:THR:CA | 1:231:C:THR:C | 1:232:C:PRO:N | 5 | 2.03 |
| (1,65) | 1:207:C:TYR:C | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 19 | 2.03 |
| (1,36) | 1:39:A:VAL:N | 1:39:A:VAL:CA | 1:39:A:VAL:C | 1:40:A:ALA:N | 6 | 2.02 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 13 | 2.02 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 6 | 2.01 |
| (1,39) | 1:40:A:ALA:C | 1:41:A:ARG:N | 1:41:A:ARG:CA | 1:41:A:ARG:C | 19 | 2.0 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 12 | 1.99 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 4 | 1.98 |
| (1,94) | 1:231:C:THR:N | 1:231:C:THR:CA | 1:231:C:THR:C | 1:232:C:PRO:N | 3 | 1.95 |
| (1,91) | 1:229:C:LEU:C | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 14 | 1.94 |
| (1,29) | 1:30:A:ASN:C | 1:31:A:THR:N | 1:31:A:THR:CA | 1:31:A:THR:C | 5 | 1.94 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 19 | 1.93 |
| (1,114) | 1:257:C:TRP:N | 1:257:C:TRP:CA | 1:257:C:TRP:C | 1:258:C:ILE:N | 13 | 1.9 |
| (1,57) | 1:60:A:GLU:C | 1:61:A:TYR:N | 1:61:A:TYR:CA | 1:61:A:TYR:C | 18 | 1.9 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 11 | 1.89 |
| (1,105) | 1:247:C:ARG:C | 1:248:C:GLN:N | 1:248:C:GLN:CA | 1:248:C:GLN:C | 12 | 1.89 |
| (1,75) | 1:214:C:PHE:C | 1:215:C:GLU:N | 1:215:C:GLU:CA | 1:215:C:GLU:C | 7 | 1.89 |
| (1,19) | 1:22:A:ASN:C | 1:23:A:VAL:N | 1:23:A:VAL:CA | 1:23:A:VAL:C | 4 | 1.89 |
| (1,92) | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 1:231:C:THR:N | 16 | 1.88 |
| (1,12) | 1:15:A:GLU:N | 1:15:A:GLU:CA | 1:15:A:GLU:C | 1:16:A:SER:N | 16 | 1.88 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 2 | 1.87 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 2 | 1.87 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 15 | 1.85 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 5 | 1.85 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 20 | 1.84 |
| (1,95) | 1:233:C:ASN:C | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 14 | 1.84 |
| (1,75) | 1:214:C:PHE:C | 1:215:C:GLU:N | 1:215:C:GLU:CA | 1:215:C:GLU:C | 9 | 1.84 |
| (1,9) | 1:13:A:PHE:C | 1:14:A:PHE:N | 1:14:A:PHE:CA | 1:14:A:PHE:C | 14 | 1.84 |
| (1,82) | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 1:222:C:ASN:N | 7 | 1.83 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 10 | 1.83 |
| (1,108) | 1:249:C:VAL:N | 1:249:C:VAL:CA | 1:249:C:VAL:C | 1:250:C:CYS:N | 16 | 1.82 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 13 | 1.82 |
| (1,18) | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1:22:A:ASN:N | 5 | 1.82 |
| (1,10) | 1:14:A:PHE:N | 1:14:A:PHE:CA | 1:14:A:PHE:C | 1:15:A:GLU:N | 12 | 1.82 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 16 | 1.81 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 8 | 1.8 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 11 | 1.78 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 8 | 1.78 |
| (1,56) | 1:60:A:GLU:N | 1:60:A:GLU:CA | 1:60:A:GLU:C | 1:61:A:TYR:N | 15 | 1.77 |
| (1,17) | 1:20:A:ARG:C | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 16 | 1.77 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 17 | 1.75 |
| (1,89) | 1:227:C:LYS:C | 1:228:C:ILE:N | 1:228:C:ILE:CA | 1:228:C:ILE:C | 19 | 1.72 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 10 | 1.72 |
| (1,19) | 1:22:A:ASN:C | 1:23:A:VAL:N | 1:23:A:VAL:CA | 1:23:A:VAL:C | 9 | 1.72 |
| (1,95) | 1:233:C:ASN:C | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1 | 1.71 |
| (1,121) | 1:260:C:GLU:C | 1:261:C:TYR:N | 1:261:C:TYR:CA | 1:261:C:TYR:C | 18 | 1.7 |
| (1,83) | 1:222:C:ASN:C | 1:223:C:VAL:N | 1:223:C:VAL:CA | 1:223:C:VAL:C | 14 | 1.7 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 7 | 1.7 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 14 | 1.7 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 11 | 1.7 |
| (1,17) | 1:20:A:ARG:C | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 20 | 1.69 |
| (1,1) | 1:7:A:TYR:C | 1:8:A:ARG:N | 1:8:A:ARG:CA | 1:8:A:ARG:C | 7 | 1.69 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 9 | 1.67 |
| (1,95) | 1:233:C:ASN:C | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 10 | 1.66 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 12 | 1.64 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 9 | 1.64 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 7 | 1.63 |
| (1,61) | 1:62:A:LEU:C | 1:63:A:GLU:N | 1:63:A:GLU:CA | 1:63:A:GLU:C | 10 | 1.63 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 11 | 1.61 |
| (1,56) | 1:60:A:GLU:N | 1:60:A:GLU:CA | 1:60:A:GLU:C | 1:61:A:TYR:N | 18 | 1.61 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 18 | 1.61 |
| (1,100) | 1:239:C:VAL:N | 1:239:C:VAL:CA | 1:239:C:VAL:C | 1:240:C:ALA:N | 14 | 1.6 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 3 | 1.59 |
| (1,82) | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 1:222:C:ASN:N | 1 | 1.59 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 17 | 1.59 |
| (1,3) | 1:8:A:ARG:C | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 2 | 1.57 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 14 | 1.56 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 4 | 1.55 |
| (1,31) | 1:33:A:ASN:C | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 16 | 1.55 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 1 | 1.54 |
| (1,12) | 1:15:A:GLU:N | 1:15:A:GLU:CA | 1:15:A:GLU:C | 1:16:A:SER:N | 13 | 1.54 |
| (1,39) | 1:40:A:ALA:C | 1:41:A:ARG:N | 1:41:A:ARG:CA | 1:41:A:ARG:C | 9 | 1.53 |
| (1,14) | 1:19:A:ALA:N | 1:19:A:ALA:CA | 1:19:A:ALA:C | 1:20:A:ARG:N | 3 | 1.53 |
| (1,106) | 1:248:C:GLN:N | 1:248:C:GLN:CA | 1:248:C:GLN:C | 1:249:C:VAL:N | 8 | 1.52 |
| (1,88) | 1:227:C:LYS:N | 1:227:C:LYS:CA | 1:227:C:LYS:C | 1:228:C:ILE:N | 5 | 1.51 |
| (1,40) | 1:41:A:ARG:N | 1:41:A:ARG:CA | 1:41:A:ARG:C | 1:42:A:LEU:N | 6 | 1.51 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 13 | 1.5 |
| (1,24) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:ILE:N | 5 | 1.5 |
| (1,9) | 1:13:A:PHE:C | 1:14:A:PHE:N | 1:14:A:PHE:CA | 1:14:A:PHE:C | 4 | 1.5 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 4 | 1.48 |
| (1,24) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:ILE:N | 20 | 1.48 |
| (1,73) | 1:213:C:PHE:C | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 13 | 1.46 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 18 | 1.46 |
| (1,13) | 1:18:A:VAL:C | 1:19:A:ALA:N | 1:19:A:ALA:CA | 1:19:A:ALA:C | 3 | 1.45 |
| (1,54) | 1:59:A:GLN:N | 1:59:A:GLN:CA | 1:59:A:GLN:C | 1:60:A:GLU:N | 13 | 1.44 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 6 | 1.44 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 8 | 1.44 |
| (1,2) | 1:8:A:ARG:N | 1:8:A:ARG:CA | 1:8:A:ARG:C | 1:9:A:CYS:N | 11 | 1.44 |
| (1,111) | 1:250:C:CYS:C | 1:251:C:ILE:N | 1:251:C:ILE:CA | 1:251:C:ILE:C | 10 | 1.43 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 8 | 1.43 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 8 | 1.42 |
| (1,81) | 1:220:C:ARG:C | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 17 | 1.42 |
| (1,54) | 1:59:A:GLN:N | 1:59:A:GLN:CA | 1:59:A:GLN:C | 1:60:A:GLU:N | 2 | 1.42 |
| (1,2) | 1:8:A:ARG:N | 1:8:A:ARG:CA | 1:8:A:ARG:C | 1:9:A:CYS:N | 6 | 1.42 |
| (1,89) | 1:227:C:LYS:C | 1:228:C:ILE:N | 1:228:C:ILE:CA | 1:228:C:ILE:C | 8 | 1.41 |
| (1,31) | 1:33:A:ASN:C | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 3 | 1.41 |
| (1,120) | 1:260:C:GLU:N | 1:260:C:GLU:CA | 1:260:C:GLU:C | 1:261:C:TYR:N | 11 | 1.39 |
| (1,128) | 1:264:C:LYS:N | 1:264:C:LYS:CA | 1:264:C:LYS:C | 1:265:C:CYS:N | 11 | 1.38 |
| (1,120) | 1:260:C:GLU:N | 1:260:C:GLU:CA | 1:260:C:GLU:C | 1:261:C:TYR:N | 20 | 1.38 |
| (1,114) | 1:257:C:TRP:N | 1:257:C:TRP:CA | 1:257:C:TRP:C | 1:258:C:ILE:N | 15 | 1.38 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 20 | 1.38 |
| (1,66) | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 1:209:C:CYS:N | 4 | 1.38 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 2 | 1.38 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 17 | 1.37 |
| (1,88) | 1:227:C:LYS:N | 1:227:C:LYS:CA | 1:227:C:LYS:C | 1:228:C:ILE:N | 15 | 1.36 |
| (1,82) | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 1:222:C:ASN:N | 11 | 1.36 |
| (1,105) | 1:247:C:ARG:C | 1:248:C:GLN:N | 1:248:C:GLN:CA | 1:248:C:GLN:C | 6 | 1.35 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 20 | 1.35 |
| (1,18) | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1:22:A:ASN:N | 13 | 1.35 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 2 | 1.35 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 13 | 1.35 |
| (1,83) | 1:222:C:ASN:C | 1:223:C:VAL:N | 1:223:C:VAL:CA | 1:223:C:VAL:C | 1 | 1.34 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 6 | 1.32 |
| (1,83) | 1:222:C:ASN:C | 1:223:C:VAL:N | 1:223:C:VAL:CA | 1:223:C:VAL:C | 2 | 1.32 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 2 | 1.32 |
| (1,18) | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1:22:A:ASN:N | 17 | 1.32 |
| (1,105) | 1:247:C:ARG:C | 1:248:C:GLN:N | 1:248:C:GLN:CA | 1:248:C:GLN:C | 7 | 1.31 |
| (1,89) | 1:227:C:LYS:C | 1:228:C:ILE:N | 1:228:C:ILE:CA | 1:228:C:ILE:C | 11 | 1.31 |
| (1,56) | 1:60:A:GLU:N | 1:60:A:GLU:CA | 1:60:A:GLU:C | 1:61:A:TYR:N | 20 | 1.31 |
| (1,19) | 1:22:A:ASN:C | 1:23:A:VAL:N | 1:23:A:VAL:CA | 1:23:A:VAL:C | 18 | 1.31 |
| (1,3) | 1:8:A:ARG:C | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 18 | 1.31 |
| (1,84) | 1:223:C:VAL:N | 1:223:C:VAL:CA | 1:223:C:VAL:C | 1:224:C:LYS:N | 16 | 1.3 |
| (1,72) | 1:213:C:PHE:N | 1:213:C:PHE:CA | 1:213:C:PHE:C | 1:214:C:PHE:N | 14 | 1.3 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 5 | 1.3 |
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 9 | 1.3 |
| (1,94) | 1:231:C:THR:N | 1:231:C:THR:CA | 1:231:C:THR:C | 1:232:C:PRO:N | 7 | 1.29 |
| (1,73) | 1:213:C:PHE:C | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 17 | 1.29 |
| (1,42) | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 1:49:A:VAL:N | 16 | 1.28 |
| (1,16) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:ALA:N | 15 | 1.28 |
| (1,114) | 1:257:C:TRP:N | 1:257:C:TRP:CA | 1:257:C:TRP:C | 1:258:C:ILE:N | 19 | 1.27 |
| (1,91) | 1:229:C:LEU:C | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 16 | 1.27 |
| (1,65) | 1:207:C:TYR:C | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 10 | 1.27 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 7 | 1.26 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 11 | 1.26 |
| (1,85) | 1:225:C:HIS:C | 1:226:C:LEU:N | 1:226:C:LEU:CA | 1:226:C:LEU:C | 20 | 1.26 |
| (1,76) | 1:215:C:GLU:N | 1:215:C:GLU:CA | 1:215:C:GLU:C | 1:216:C:SER:N | 15 | 1.26 |
| (1,68) | 1:209:C:CYS:N | 1:209:C:CYS:CA | 1:209:C:CYS:C | 1:210:C:PRO:N | 4 | 1.26 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,65) | 1:207:C:TYR:C | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 1 | 1.26 |
| (1,44) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:CYS:N | 4 | 1.26 |
| (1,34) | 1:38:A:ILE:N | 1:38:A:ILE:CA | 1:38:A:ILE:C | 1:39:A:VAL:N | 8 | 1.26 |
| (1,29) | 1:30:A:ASN:C | 1:31:A:THR:N | 1:31:A:THR:CA | 1:31:A:THR:C | 18 | 1.26 |
| (1,20) | 1:23:A:VAL:N | 1:23:A:VAL:CA | 1:23:A:VAL:C | 1:24:A:LYS:N | 12 | 1.26 |
| (1,1) | 1:7:A:TYR:C | 1:8:A:ARG:N | 1:8:A:ARG:CA | 1:8:A:ARG:C | 20 | 1.26 |
| (1,110) | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 1:251:C:ILE:N | 5 | 1.25 |
| (1,114) | 1:257:C:TRP:N | 1:257:C:TRP:CA | 1:257:C:TRP:C | 1:258:C:ILE:N | 18 | 1.24 |
| (1,81) | 1:220:C:ARG:C | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 12 | 1.24 |
| (1,80) | 1:220:C:ARG:N | 1:220:C:ARG:CA | 1:220:C:ARG:C | 1:221:C:ALA:N | 13 | 1.24 |
| (1,95) | 1:233:C:ASN:C | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 13 | 1.23 |
| (1,92) | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 1:231:C:THR:N | 9 | 1.23 |
| (1,83) | 1:222:C:ASN:C | 1:223:C:VAL:N | 1:223:C:VAL:CA | 1:223:C:VAL:C | 6 | 1.23 |
| (1,18) | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1:22:A:ASN:N | 12 | 1.23 |
| (1,3) | 1:8:A:ARG:C | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 15 | 1.23 |
| (1,103) | 1:240:C:ALA:C | 1:241:C:ARG:N | 1:241:C:ARG:CA | 1:241:C:ARG:C | 20 | 1.22 |
| (1,21) | 1:25:A:HIS:C | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C | 12 | 1.22 |
| (1,85) | 1:225:C:HIS:C | 1:226:C:LEU:N | 1:226:C:LEU:CA | 1:226:C:LEU:C | 6 | 1.21 |
| (1,85) | 1:225:C:HIS:C | 1:226:C:LEU:N | 1:226:C:LEU:CA | 1:226:C:LEU:C | 11 | 1.21 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 1 | 1.21 |
| (1,27) | 1:29:A:LEU:C | 1:30:A:ASN:N | 1:30:A:ASN:CA | 1:30:A:ASN:C | 12 | 1.21 |
| (1,105) | 1:247:C:ARG:C | 1:248:C:GLN:N | 1:248:C:GLN:CA | 1:248:C:GLN:C | 13 | 1.2 |
| (1,95) | 1:233:C:ASN:C | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 16 | 1.2 |
| (1,73) | 1:213:C:PHE:C | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 7 | 1.2 |
| (1,73) | 1:213:C:PHE:C | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 6 | 1.19 |
| (1,18) | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1:22:A:ASN:N | 18 | 1.19 |
| (1,5) | 1:10:A:PRO:C | 1:11:A:CYS:N | 1:11:A:CYS:CA | 1:11:A:CYS:C | 11 | 1.19 |
| (1,96) | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 1:235:C:ALA:N | 12 | 1.18 |
| (1,40) | 1:41:A:ARG:N | 1:41:A:ARG:CA | 1:41:A:ARG:C | 1:42:A:LEU:N | 16 | 1.18 |
| (1,85) | 1:225:C:HIS:C | 1:226:C:LEU:N | 1:226:C:LEU:CA | 1:226:C:LEU:C | 12 | 1.17 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 19 | 1.17 |
| (1,31) | 1:33:A:ASN:C | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 8 | 1.17 |
| (1,17) | 1:20:A:ARG:C | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 6 | 1.17 |
| (1,15) | 1:19:A:ALA:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 11 | 1.17 |
| (1,114) | 1:257:C:TRP:N | 1:257:C:TRP:CA | 1:257:C:TRP:C | 1:258:C:ILE:N | 11 | 1.16 |
| (1,93) | 1:230:C:ASN:C | 1:231:C:THR:N | 1:231:C:THR:CA | 1:231:C:THR:C | 19 | 1.15 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 2 | 1.15 |
| (1,38) | 1:40:A:ALA:N | 1:40:A:ALA:CA | 1:40:A:ALA:C | 1:41:A:ARG:N | 19 | 1.15 |
| (1,128) | 1:264:C:LYS:N | 1:264:C:LYS:CA | 1:264:C:LYS:C | 1:265:C:CYS:N | 18 | 1.13 |
| (1,95) | 1:233:C:ASN:C | 1:234:C:CYS:N | 1:234:C:CYS:CA | 1:234:C:CYS:C | 3 | 1.13 |
| (1,89) | 1:227:C:LYS:C | 1:228:C:ILE:N | 1:228:C:ILE:CA | 1:228:C:ILE:C | 16 | 1.13 |
| (1,114) | 1:257:C:TRP:N | 1:257:C:TRP:CA | 1:257:C:TRP:C | 1:258:C:ILE:N | 16 | 1.12 |
| (1,35) | 1:38:A:ILE:C | 1:39:A:VAL:N | 1:39:A:VAL:CA | 1:39:A:VAL:C | 9 | 1.12 |
| (1,124) | 1:262:C:LEU:N | 1:262:C:LEU:CA | 1:262:C:LEU:C | 1:263:C:GLU:N | 12 | 1.11 |
| (1,94) | 1:231:C:THR:N | 1:231:C:THR:CA | 1:231:C:THR:C | 1:232:C:PRO:N | 18 | 1.11 |
| (1,66) | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 1:209:C:CYS:N | 2 | 1.11 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 15 | 1.11 |
| (1,28) | 1:30:A:ASN:N | 1:30:A:ASN:CA | 1:30:A:ASN:C | 1:31:A:THR:N | 7 | 1.11 |
| (1,27) | 1:29:A:LEU:C | 1:30:A:ASN:N | 1:30:A:ASN:CA | 1:30:A:ASN:C | 20 | 1.11 |
| (1,18) | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1:22:A:ASN:N | 16 | 1.11 |
| (1,127) | 1:263:C:GLU:C | 1:264:C:LYS:N | 1:264:C:LYS:CA | 1:264:C:LYS:C | 4 | 1.1 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---|---|---|---|---|---|---|
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 19 | 1.1 |
| (1,125) | 1:262:C:LEU:C | 1:263:C:GLU:N | 1:263:C:GLU:CA | 1:263:C:GLU:C | 19 | 1.09 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 6 | 1.09 |
| (1,24) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:ILE:N | 19 | 1.09 |
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 13 | 1.09 |
| (1,99) | 1:238:C:ILE:C | 1:239:C:VAL:N | 1:239:C:VAL:CA | 1:239:C:VAL:C | 7 | 1.08 |
| (1,94) | 1:231:C:THR:N | 1:231:C:THR:CA | 1:231:C:THR:C | 1:232:C:PRO:N | 15 | 1.08 |
| (1,74) | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 1:215:C:GLU:N | 2 | 1.08 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 9 | 1.08 |
| (1,17) | 1:20:A:ARG:C | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 8 | 1.08 |
| (1,15) | 1:19:A:ALA:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 17 | 1.08 |
| (1,92) | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 1:231:C:THR:N | 6 | 1.07 |
| (1,74) | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 1:215:C:GLU:N | 19 | 1.07 |
| (1,54) | 1:59:A:GLN:N | 1:59:A:GLN:CA | 1:59:A:GLN:C | 1:60:A:GLU:N | 9 | 1.07 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 4 | 1.07 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 4 | 1.06 |
| (1,30) | 1:31:A:THR:N | 1:31:A:THR:CA | 1:31:A:THR:C | 1:32:A:PRO:N | 16 | 1.06 |
| (1,16) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:ALA:N | 3 | 1.06 |
| (1,3) | 1:8:A:ARG:C | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 3 | 1.06 |
| (1,94) | 1:231:C:THR:N | 1:231:C:THR:CA | 1:231:C:THR:C | 1:232:C:PRO:N | 8 | 1.05 |
| (1,85) | 1:225:C:HIS:C | 1:226:C:LEU:N | 1:226:C:LEU:CA | 1:226:C:LEU:C | 16 | 1.05 |
| (1,54) | 1:59:A:GLN:N | 1:59:A:GLN:CA | 1:59:A:GLN:C | 1:60:A:GLU:N | 12 | 1.05 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 5 | 1.04 |
| (1,40) | 1:41:A:ARG:N | 1:41:A:ARG:CA | 1:41:A:ARG:C | 1:42:A:LEU:N | 12 | 1.04 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 15 | 1.04 |
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 1 | 1.04 |
| (1,103) | 1:240:C:ALA:C | 1:241:C:ARG:N | 1:241:C:ARG:CA | 1:241:C:ARG:C | 8 | 1.03 |
| (1,82) | 1:221:C:ALA:N | 1:221:C:ALA:CA | 1:221:C:ALA:C | 1:222:C:ASN:N | 10 | 1.03 |
| (1,69) | 1:210:C:PRO:C | 1:211:C:CYS:N | 1:211:C:CYS:CA | 1:211:C:CYS:C | 15 | 1.03 |
| (1,24) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:ILE:N | 15 | 1.03 |
| (1,2) | 1:8:A:ARG:N | 1:8:A:ARG:CA | 1:8:A:ARG:C | 1:9:A:CYS:N | 17 | 1.03 |
| (1,128) | 1:264:C:LYS:N | 1:264:C:LYS:CA | 1:264:C:LYS:C | 1:265:C:CYS:N | 2 | 1.02 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 4 | 1.02 |
| (1,74) | 1:214:C:PHE:N | 1:214:C:PHE:CA | 1:214:C:PHE:C | 1:215:C:GLU:N | 8 | 1.02 |
| (1,66) | 1:208:C:ARG:N | 1:208:C:ARG:CA | 1:208:C:ARG:C | 1:209:C:CYS:N | 17 | 1.02 |
| (1,41) | 1:47:A:ARG:C | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C | 20 | 1.02 |
| (1,32) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C | 1:35:A:ALA:N | 20 | 1.02 |
| (1,21) | 1:25:A:HIS:C | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C | 10 | 1.02 |
| (1,4) | 1:9:A:CYS:N | 1:9:A:CYS:CA | 1:9:A:CYS:C | 1:10:A:PRO:N | 12 | 1.02 |
| (1,104) | 1:241:C:ARG:N | 1:241:C:ARG:CA | 1:241:C:ARG:C | 1:242:C:LEU:N | 13 | 1.01 |
| (1,91) | 1:229:C:LEU:C | 1:230:C:ASN:N | 1:230:C:ASN:CA | 1:230:C:ASN:C | 17 | 1.01 |
| (1,12) | 1:15:A:GLU:N | 1:15:A:GLU:CA | 1:15:A:GLU:C | 1:16:A:SER:N | 12 | 1.01 |
| (1,118) | 1:259:C:GLN:N | 1:259:C:GLN:CA | 1:259:C:GLN:C | 1:260:C:GLU:N | 20 | 1.0 |
| (1,110) | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 1:251:C:ILE:N | 12 | 1.0 |
| (1,109) | 1:249:C:VAL:C | 1:250:C:CYS:N | 1:250:C:CYS:CA | 1:250:C:CYS:C | 14 | 1.0 |
| (1,62) | 1:63:A:GLU:N | 1:63:A:GLU:CA | 1:63:A:GLU:C | 1:64:A:LYS:N | 15 | 1.0 |
| (1,50) | 1:57:A:TRP:N | 1:57:A:TRP:CA | 1:57:A:TRP:C | 1:58:A:ILE:N | 9 | 1.0 |
| (1,45) | 1:49:A:VAL:C | 1:50:A:CYS:N | 1:50:A:CYS:CA | 1:50:A:CYS:C | 8 | 1.0 |
| (1,30) | 1:31:A:THR:N | 1:31:A:THR:CA | 1:31:A:THR:C | 1:32:A:PRO:N | 18 | 1.0 |
| (1,17) | 1:20:A:ARG:C | 1:21:A:ALA:N | 1:21:A:ALA:CA | 1:21:A:ALA:C | 1 | 1.0 |