



Full wwPDB NMR Structure Validation Report ⓘ

Jun 5, 2023 – 02:54 AM EDT

PDB ID : 2LSR
BMRB ID : 18441
Title : Solution structure of harmonin N terminal domain in complex with a exon68 encoded peptide of cadherin23
Authors : Pan, L.; Wu, L.; Zhang, C.; Zhang, M.
Deposited on : 2012-05-04

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

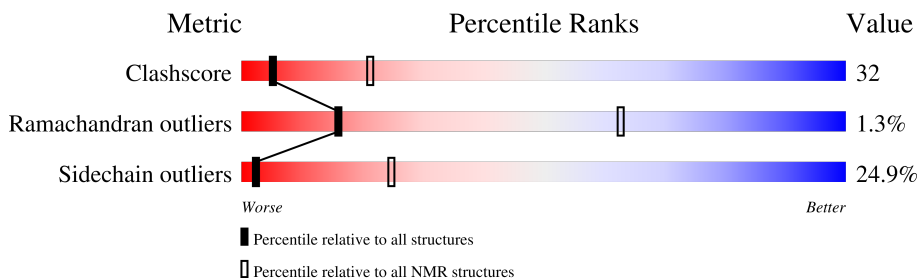
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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



| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|-----------------------|--------------------------|------------------------|
| Clashscore | 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 80 | |
| 2 | B | 16 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:3-A:74, B:100-B:107 (80) | 0.45 | 17 |

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1643 atoms, of which 837 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Harmonin.

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|-----|-----|-----|-----|-------|---|
| | | | Total | C | H | N | O | | S |
| 1 | A | 80 | 1360 | 432 | 688 | 117 | 120 | 3 | 0 |

- Molecule 2 is a protein called peptide from Cadherin-23.

| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|----|-----|----|----|-------|
| | | | Total | C | H | N | O | |
| 2 | B | 16 | 283 | 87 | 149 | 22 | 25 | 0 |

There is a discrepancy between the modelled and reference sequences:

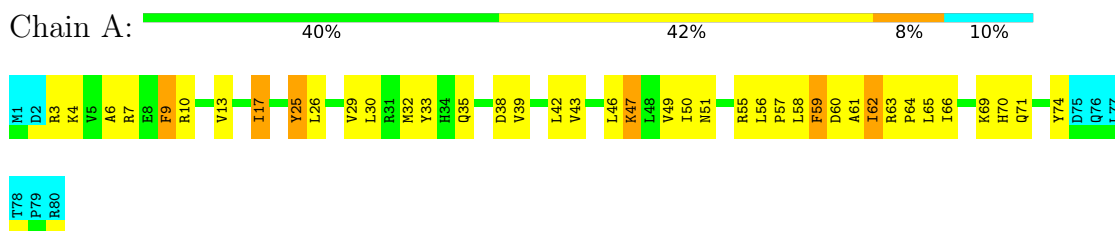
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | 103 | GLU | VAL | engineered mutation | UNP F6U049 |

4 Residue-property plots

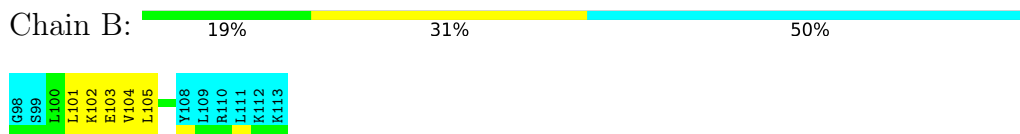
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Harmonin



- Molecule 2: peptide from Cadherin-23

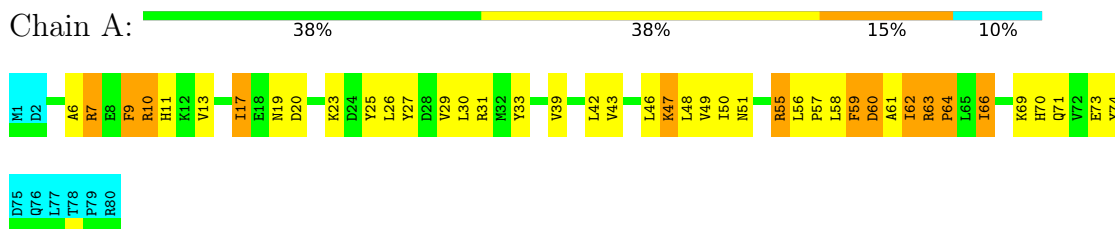


4.2 Scores per residue for each member of the ensemble

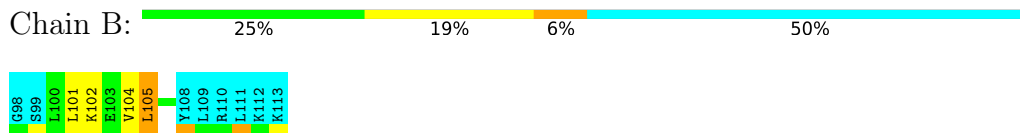
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Harmonin

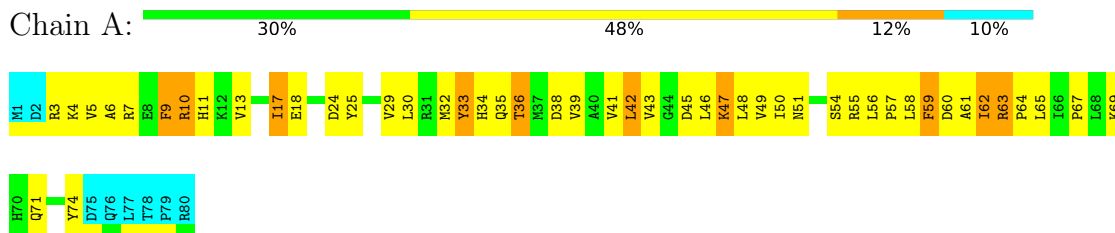


- Molecule 2: peptide from Cadherin-23

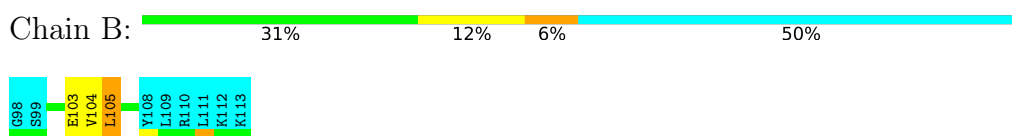


4.2.2 Score per residue for model 2

- Molecule 1: Harmonin

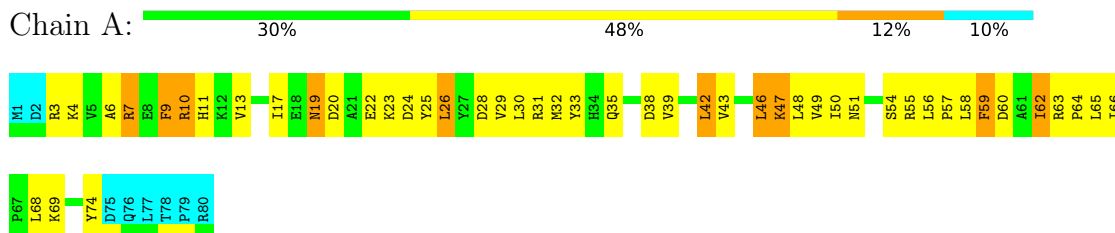


- Molecule 2: peptide from Cadherin-23

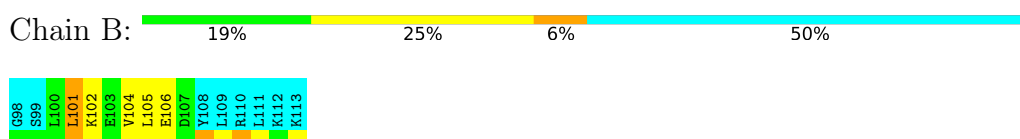


4.2.3 Score per residue for model 3

- Molecule 1: Harmonin

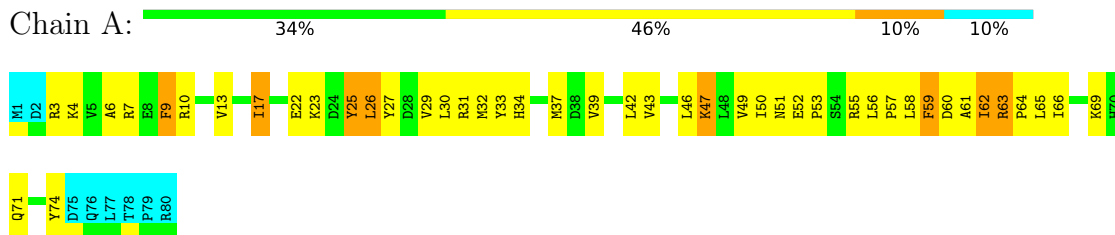


- Molecule 2: peptide from Cadherin-23



4.2.4 Score per residue for model 4

- Molecule 1: Harmonin

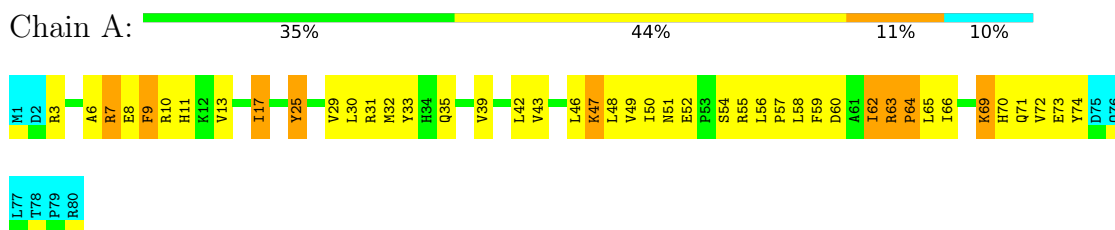


- Molecule 2: peptide from Cadherin-23



4.2.5 Score per residue for model 5

- Molecule 1: Harmonin

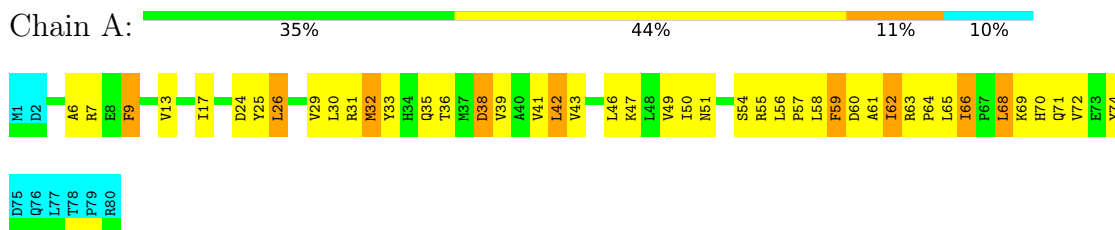


- Molecule 2: peptide from Cadherin-23



4.2.6 Score per residue for model 6

- Molecule 1: Harmonin



- Molecule 2: peptide from Cadherin-23

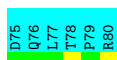




4.2.7 Score per residue for model 7

- Molecule 1: Harmonin

Chain A: 39% 42% 9% 10%



- Molecule 2: peptide from Cadherin-23

Chain B: 12% 25% 12% 50%



4.2.8 Score per residue for model 8

- Molecule 1: Harmonin

Chain A: 40% 41% 9% 10%



- Molecule 2: peptide from Cadherin-23

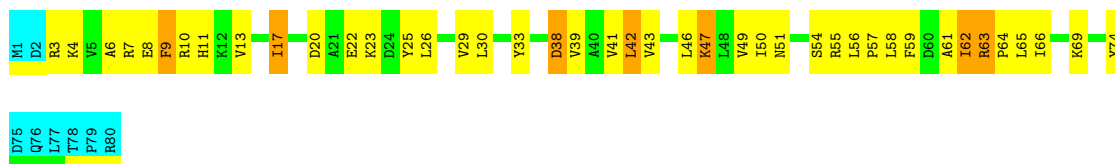
Chain B: 12% 31% 6% 50%



4.2.9 Score per residue for model 9

- Molecule 1: Harmonin

Chain A: 38% 44% 9% 10%

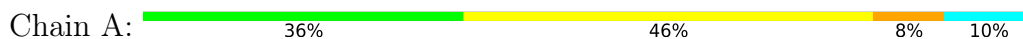


- Molecule 2: peptide from Cadherin-23

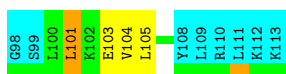


4.2.10 Score per residue for model 10

- Molecule 1: Harmonin

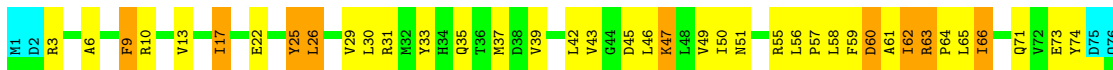


- Molecule 2: peptide from Cadherin-23



4.2.11 Score per residue for model 11

- Molecule 1: Harmonin



- Molecule 2: peptide from Cadherin-23

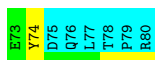
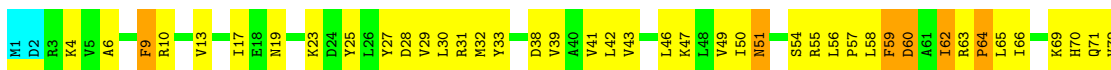




4.2.12 Score per residue for model 12

- Molecule 1: Harmonin

Chain A: 36% 46% 8% 10%



- Molecule 2: peptide from Cadherin-23

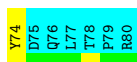
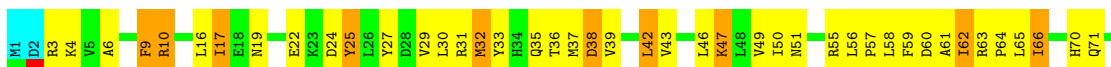
Chain B: 19% 25% 6% 50%



4.2.13 Score per residue for model 13

- Molecule 1: Harmonin

Chain A: 35% 42% 12% 10%



- Molecule 2: peptide from Cadherin-23

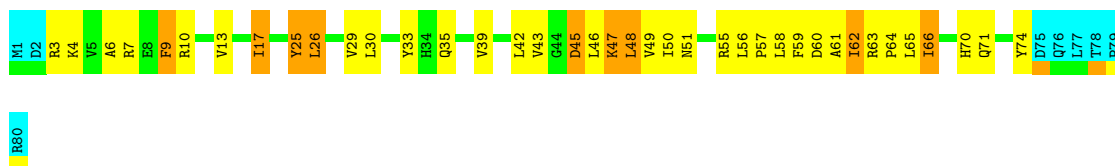
Chain B: 19% 31% 50%



4.2.14 Score per residue for model 14

- Molecule 1: Harmonin

Chain A: 41% 38% 11% 10%

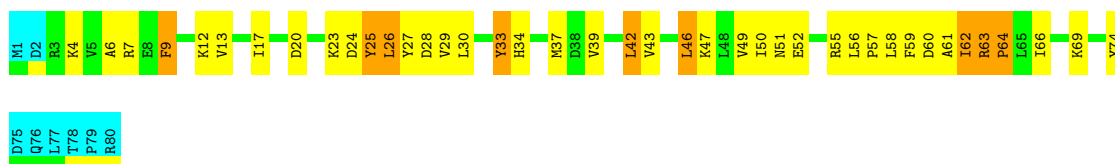


- Molecule 2: peptide from Cadherin-23



4.2.15 Score per residue for model 15

- Molecule 1: Harmonin

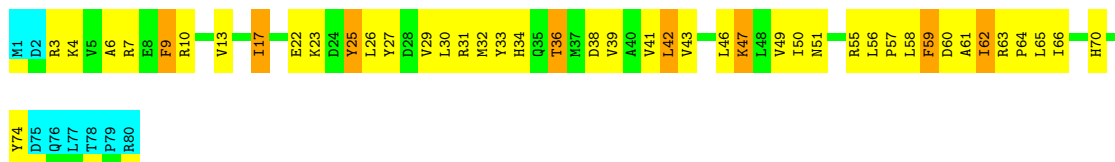
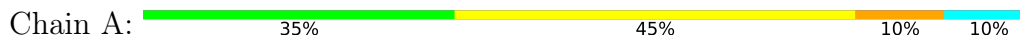


- Molecule 2: peptide from Cadherin-23

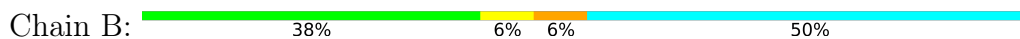


4.2.16 Score per residue for model 16

- Molecule 1: Harmonin



- Molecule 2: peptide from Cadherin-23

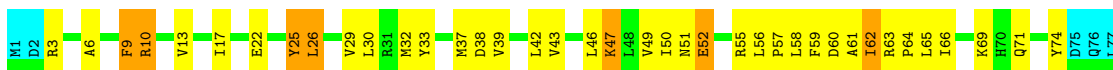




4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Harmonin

Chain A: 41% 40% 9% 10%



- Molecule 2: peptide from Cadherin-23

Chain B: 19% 25% 6% 50%



4.2.18 Score per residue for model 18

- Molecule 1: Harmonin

Chain A: 40% 39% 11% 10%



- Molecule 2: peptide from Cadherin-23

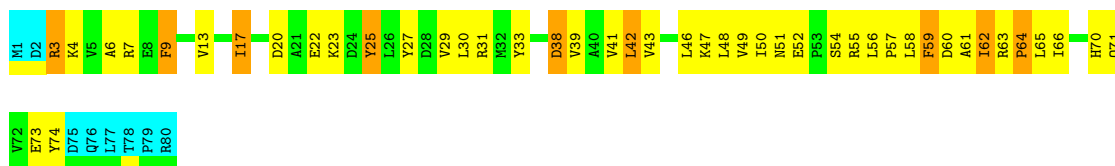
Chain B: 12% 38% 50%



4.2.19 Score per residue for model 19

- Molecule 1: Harmonin

Chain A: 34% 45% 11% 10%

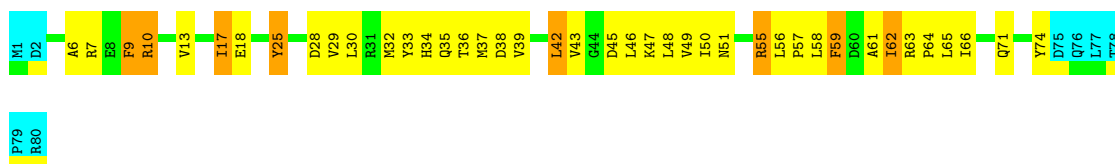
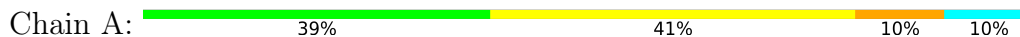


- Molecule 2: peptide from Cadherin-23



4.2.20 Score per residue for model 20

- Molecule 1: Harmonin



- Molecule 2: peptide from Cadherin-23



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CNS | structure solution | |
| CNS | refinement | |

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

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1132 |
| Number of shifts mapped to atoms | 1132 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 81% |

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 606 | 623 | 620 | 43±5 |
| 2 | B | 66 | 71 | 71 | 6±2 |
| All | All | 13440 | 13880 | 13820 | 876 |

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 32.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 1.14 | 1.20 | 7 | 20 |
| 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 1.10 | 1.22 | 6 | 20 |
| 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 0.87 | 1.46 | 17 | 6 |
| 1:A:29:VAL:HG12 | 1:A:42:LEU:HD13 | 0.86 | 1.45 | 3 | 1 |
| 1:A:29:VAL:HG12 | 1:A:42:LEU:HD23 | 0.86 | 1.47 | 8 | 8 |
| 1:A:33:TYR:CD2 | 2:B:101:LEU:HD13 | 0.86 | 2.06 | 7 | 3 |
| 1:A:17:ILE:HD11 | 1:A:58:LEU:HD11 | 0.85 | 1.45 | 6 | 1 |
| 1:A:9:PHE:CD1 | 1:A:61:ALA:HB1 | 0.84 | 2.07 | 8 | 12 |
| 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 0.83 | 1.50 | 18 | 7 |
| 1:A:6:ALA:CB | 2:B:104:VAL:HG22 | 0.82 | 2.03 | 19 | 13 |
| 1:A:25:TYR:O | 1:A:29:VAL:HG23 | 0.81 | 1.76 | 11 | 20 |
| 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 0.80 | 1.52 | 8 | 3 |
| 1:A:39:VAL:O | 1:A:43:VAL:HG23 | 0.80 | 1.77 | 13 | 20 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:50:ILE:HG23 | 1:A:55:ARG:O | 0.80 | 1.77 | 7 | 20 |
| 1:A:30:LEU:CD2 | 1:A:62:ILE:HD11 | 0.77 | 2.08 | 14 | 17 |
| 1:A:29:VAL:CG1 | 1:A:42:LEU:HD23 | 0.76 | 2.09 | 18 | 5 |
| 1:A:13:VAL:HG22 | 1:A:58:LEU:CD2 | 0.75 | 2.11 | 1 | 13 |
| 1:A:46:LEU:HD22 | 1:A:50:ILE:CD1 | 0.75 | 2.10 | 6 | 8 |
| 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 0.74 | 1.58 | 17 | 8 |
| 1:A:9:PHE:CE2 | 1:A:65:LEU:HD11 | 0.73 | 2.18 | 19 | 13 |
| 1:A:50:ILE:HG22 | 1:A:50:ILE:O | 0.73 | 1.82 | 4 | 20 |
| 1:A:30:LEU:HD21 | 1:A:62:ILE:CD1 | 0.71 | 2.14 | 18 | 5 |
| 1:A:33:TYR:CD2 | 2:B:101:LEU:HD22 | 0.70 | 2.22 | 12 | 3 |
| 1:A:6:ALA:HB1 | 2:B:104:VAL:CG2 | 0.70 | 2.13 | 15 | 12 |
| 1:A:13:VAL:HG13 | 1:A:58:LEU:CD2 | 0.69 | 2.17 | 9 | 10 |
| 1:A:9:PHE:CZ | 2:B:104:VAL:HG11 | 0.69 | 2.22 | 20 | 18 |
| 1:A:42:LEU:O | 1:A:46:LEU:HD12 | 0.69 | 1.88 | 3 | 2 |
| 1:A:29:VAL:HG12 | 1:A:42:LEU:CD2 | 0.68 | 2.18 | 11 | 8 |
| 1:A:62:ILE:HG13 | 1:A:65:LEU:HD12 | 0.68 | 1.65 | 8 | 9 |
| 1:A:68:LEU:O | 1:A:72:VAL:HG23 | 0.67 | 1.90 | 6 | 1 |
| 1:A:43:VAL:HG22 | 1:A:74:TYR:CE1 | 0.67 | 2.25 | 20 | 2 |
| 1:A:39:VAL:HG11 | 1:A:74:TYR:HB2 | 0.66 | 1.68 | 1 | 1 |
| 1:A:29:VAL:HG11 | 1:A:46:LEU:HG | 0.66 | 1.67 | 5 | 10 |
| 1:A:30:LEU:HD23 | 2:B:101:LEU:HD11 | 0.66 | 1.66 | 17 | 3 |
| 1:A:46:LEU:HD22 | 1:A:50:ILE:HD12 | 0.66 | 1.65 | 6 | 4 |
| 1:A:32:MET:CE | 1:A:36:THR:HG21 | 0.66 | 2.21 | 6 | 1 |
| 1:A:33:TYR:CG | 1:A:42:LEU:HD22 | 0.65 | 2.27 | 6 | 7 |
| 1:A:17:ILE:HD11 | 1:A:58:LEU:CD1 | 0.65 | 2.21 | 6 | 1 |
| 1:A:17:ILE:HG22 | 1:A:17:ILE:O | 0.65 | 1.92 | 9 | 20 |
| 1:A:9:PHE:HB2 | 1:A:61:ALA:HB1 | 0.64 | 1.67 | 19 | 6 |
| 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 0.64 | 1.67 | 16 | 8 |
| 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 0.64 | 1.70 | 18 | 2 |
| 1:A:46:LEU:HD23 | 1:A:50:ILE:CD1 | 0.63 | 2.24 | 3 | 2 |
| 1:A:38:ASP:O | 1:A:42:LEU:HD12 | 0.63 | 1.94 | 16 | 2 |
| 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 0.63 | 1.70 | 7 | 9 |
| 1:A:43:VAL:HG22 | 1:A:74:TYR:CE2 | 0.62 | 2.29 | 4 | 3 |
| 1:A:29:VAL:HG13 | 1:A:42:LEU:HA | 0.60 | 1.73 | 20 | 9 |
| 1:A:56:LEU:N | 1:A:57:PRO:HD2 | 0.60 | 2.11 | 11 | 18 |
| 1:A:17:ILE:HG23 | 1:A:22:GLU:HB2 | 0.60 | 1.73 | 3 | 9 |
| 1:A:33:TYR:CE1 | 1:A:39:VAL:HG22 | 0.59 | 2.32 | 10 | 3 |
| 1:A:50:ILE:HG21 | 1:A:59:PHE:HB2 | 0.59 | 1.74 | 19 | 4 |
| 1:A:38:ASP:HB3 | 1:A:41:VAL:HG23 | 0.58 | 1.75 | 12 | 4 |
| 1:A:42:LEU:HD12 | 1:A:46:LEU:CD1 | 0.58 | 2.29 | 6 | 3 |
| 2:B:105:LEU:HD12 | 2:B:106:GLU:N | 0.57 | 2.14 | 15 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:39:VAL:HG11 | 1:A:74:TYR:CB | 0.57 | 2.30 | 1 | 1 |
| 1:A:9:PHE:O | 1:A:13:VAL:HG23 | 0.56 | 1.99 | 10 | 11 |
| 1:A:43:VAL:HG22 | 1:A:74:TYR:CD2 | 0.56 | 2.35 | 14 | 4 |
| 1:A:39:VAL:HA | 1:A:42:LEU:HD23 | 0.56 | 1.77 | 19 | 4 |
| 1:A:9:PHE:CZ | 1:A:65:LEU:HD11 | 0.56 | 2.35 | 8 | 4 |
| 1:A:50:ILE:O | 1:A:50:ILE:CG2 | 0.56 | 2.53 | 12 | 20 |
| 2:B:100:LEU:O | 2:B:104:VAL:HG23 | 0.55 | 2.00 | 4 | 1 |
| 1:A:9:PHE:C | 1:A:9:PHE:CD1 | 0.55 | 2.79 | 19 | 12 |
| 1:A:46:LEU:HD13 | 1:A:74:TYR:OH | 0.55 | 2.02 | 17 | 4 |
| 1:A:9:PHE:CD1 | 1:A:9:PHE:C | 0.55 | 2.80 | 8 | 8 |
| 1:A:69:LYS:O | 1:A:72:VAL:HG12 | 0.55 | 2.02 | 12 | 4 |
| 1:A:42:LEU:HD22 | 1:A:46:LEU:CD1 | 0.55 | 2.29 | 8 | 1 |
| 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 0.55 | 1.78 | 12 | 1 |
| 1:A:49:VAL:HG22 | 1:A:49:VAL:O | 0.55 | 2.01 | 2 | 20 |
| 1:A:50:ILE:HG12 | 1:A:58:LEU:HD12 | 0.54 | 1.80 | 14 | 6 |
| 1:A:9:PHE:CE2 | 2:B:104:VAL:HG11 | 0.54 | 2.37 | 4 | 1 |
| 1:A:9:PHE:HE2 | 2:B:104:VAL:HG21 | 0.54 | 1.62 | 11 | 10 |
| 1:A:9:PHE:CE2 | 2:B:104:VAL:HG21 | 0.53 | 2.38 | 11 | 9 |
| 1:A:33:TYR:CG | 1:A:42:LEU:HD11 | 0.53 | 2.38 | 11 | 2 |
| 1:A:62:ILE:CG1 | 1:A:65:LEU:HD12 | 0.53 | 2.33 | 16 | 6 |
| 1:A:33:TYR:CG | 1:A:42:LEU:HD12 | 0.53 | 2.39 | 1 | 2 |
| 1:A:26:LEU:HD12 | 1:A:49:VAL:HG11 | 0.52 | 1.81 | 11 | 1 |
| 1:A:22:GLU:O | 1:A:26:LEU:HD12 | 0.52 | 2.04 | 4 | 2 |
| 1:A:42:LEU:C | 1:A:46:LEU:HD12 | 0.52 | 2.24 | 3 | 1 |
| 1:A:10:ARG:HD2 | 2:B:104:VAL:HG12 | 0.52 | 1.81 | 4 | 1 |
| 1:A:45:ASP:HA | 1:A:48:LEU:HD12 | 0.52 | 1.80 | 20 | 2 |
| 2:B:105:LEU:HD23 | 2:B:105:LEU:N | 0.52 | 2.19 | 12 | 9 |
| 1:A:34:HIS:CD2 | 2:B:101:LEU:HD23 | 0.52 | 2.39 | 4 | 1 |
| 1:A:43:VAL:HG22 | 1:A:74:TYR:CD1 | 0.52 | 2.40 | 8 | 2 |
| 1:A:32:MET:SD | 1:A:41:VAL:HG11 | 0.51 | 2.44 | 2 | 1 |
| 1:A:29:VAL:CG1 | 1:A:42:LEU:HD13 | 0.51 | 2.28 | 3 | 1 |
| 1:A:32:MET:HE2 | 1:A:36:THR:HG21 | 0.51 | 1.81 | 6 | 1 |
| 1:A:26:LEU:HD12 | 1:A:49:VAL:HG21 | 0.51 | 1.80 | 15 | 3 |
| 1:A:33:TYR:CE2 | 2:B:101:LEU:HD22 | 0.51 | 2.41 | 9 | 1 |
| 1:A:65:LEU:CD1 | 2:B:104:VAL:HG21 | 0.51 | 2.36 | 12 | 2 |
| 1:A:46:LEU:HD23 | 1:A:50:ILE:HD11 | 0.50 | 1.83 | 3 | 1 |
| 1:A:56:LEU:N | 1:A:57:PRO:CD | 0.50 | 2.74 | 9 | 15 |
| 1:A:42:LEU:HD11 | 1:A:74:TYR:HE2 | 0.50 | 1.67 | 7 | 1 |
| 1:A:26:LEU:HD23 | 1:A:49:VAL:HG11 | 0.49 | 1.85 | 6 | 1 |
| 1:A:50:ILE:HG21 | 1:A:59:PHE:CD1 | 0.49 | 2.42 | 8 | 4 |
| 1:A:32:MET:HE3 | 1:A:36:THR:HG21 | 0.49 | 1.85 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:65:LEU:HD13 | 2:B:101:LEU:HD12 | 0.49 | 1.83 | 6 | 2 |
| 1:A:10:ARG:HH21 | 1:A:13:VAL:HG11 | 0.49 | 1.67 | 16 | 1 |
| 1:A:66:ILE:HG23 | 1:A:70:HIS:HB2 | 0.49 | 1.83 | 16 | 4 |
| 1:A:9:PHE:HD1 | 1:A:61:ALA:HB1 | 0.49 | 1.64 | 17 | 1 |
| 1:A:47:LYS:O | 1:A:51:ASN:N | 0.49 | 2.46 | 4 | 20 |
| 1:A:34:HIS:HD2 | 2:B:101:LEU:HD23 | 0.49 | 1.66 | 4 | 1 |
| 1:A:33:TYR:CE2 | 2:B:101:LEU:HD13 | 0.49 | 2.43 | 19 | 1 |
| 1:A:10:ARG:HD3 | 2:B:104:VAL:HG12 | 0.49 | 1.84 | 20 | 1 |
| 1:A:66:ILE:HG23 | 1:A:70:HIS:CB | 0.48 | 2.38 | 16 | 8 |
| 1:A:33:TYR:CG | 1:A:42:LEU:CD1 | 0.48 | 2.96 | 11 | 5 |
| 1:A:38:ASP:OD2 | 1:A:41:VAL:HG23 | 0.48 | 2.07 | 2 | 1 |
| 1:A:30:LEU:HB3 | 2:B:105:LEU:HD22 | 0.48 | 1.85 | 18 | 1 |
| 1:A:59:PHE:CE1 | 1:A:74:TYR:CZ | 0.48 | 3.02 | 20 | 1 |
| 1:A:30:LEU:CG | 1:A:62:ILE:HD11 | 0.48 | 2.39 | 19 | 4 |
| 1:A:46:LEU:HD13 | 1:A:59:PHE:CE1 | 0.48 | 2.44 | 19 | 1 |
| 1:A:33:TYR:CG | 1:A:42:LEU:CD2 | 0.48 | 2.96 | 6 | 8 |
| 1:A:65:LEU:HD13 | 2:B:101:LEU:HA | 0.48 | 1.86 | 19 | 2 |
| 1:A:38:ASP:OD2 | 1:A:41:VAL:HG21 | 0.48 | 2.08 | 16 | 1 |
| 1:A:63:ARG:CB | 1:A:64:PRO:CD | 0.47 | 2.92 | 4 | 13 |
| 1:A:10:ARG:NH2 | 1:A:13:VAL:HG11 | 0.47 | 2.24 | 16 | 1 |
| 1:A:60:ASP:O | 1:A:64:PRO:CD | 0.47 | 2.62 | 6 | 16 |
| 1:A:50:ILE:HA | 1:A:55:ARG:HB3 | 0.47 | 1.85 | 8 | 3 |
| 1:A:17:ILE:HD12 | 1:A:22:GLU:CD | 0.47 | 2.30 | 11 | 1 |
| 1:A:17:ILE:HG23 | 1:A:22:GLU:CB | 0.47 | 2.39 | 9 | 1 |
| 1:A:30:LEU:HD22 | 2:B:105:LEU:HD21 | 0.47 | 1.85 | 8 | 1 |
| 1:A:33:TYR:O | 1:A:37:MET:HA | 0.47 | 2.10 | 8 | 6 |
| 1:A:30:LEU:HB3 | 2:B:105:LEU:HD21 | 0.47 | 1.87 | 20 | 1 |
| 1:A:33:TYR:HB2 | 1:A:42:LEU:HD11 | 0.47 | 1.86 | 3 | 1 |
| 1:A:39:VAL:HG21 | 1:A:70:HIS:CG | 0.46 | 2.45 | 6 | 3 |
| 1:A:46:LEU:HD22 | 1:A:50:ILE:HD11 | 0.46 | 1.86 | 14 | 3 |
| 1:A:49:VAL:HG13 | 1:A:50:ILE:HG13 | 0.46 | 1.86 | 16 | 4 |
| 1:A:26:LEU:O | 1:A:30:LEU:HD12 | 0.46 | 2.09 | 16 | 1 |
| 1:A:46:LEU:O | 1:A:50:ILE:HD12 | 0.46 | 2.10 | 8 | 1 |
| 1:A:50:ILE:HG23 | 1:A:55:ARG:C | 0.46 | 2.30 | 10 | 3 |
| 1:A:50:ILE:HG12 | 1:A:58:LEU:HB2 | 0.46 | 1.88 | 8 | 6 |
| 1:A:63:ARG:HB3 | 1:A:64:PRO:HD3 | 0.46 | 1.86 | 6 | 3 |
| 1:A:17:ILE:HD12 | 1:A:22:GLU:HB3 | 0.46 | 1.87 | 9 | 2 |
| 1:A:30:LEU:HD23 | 2:B:101:LEU:CD1 | 0.45 | 2.38 | 17 | 1 |
| 1:A:42:LEU:CD1 | 1:A:46:LEU:HD12 | 0.45 | 2.41 | 9 | 6 |
| 1:A:65:LEU:CD1 | 2:B:101:LEU:HD12 | 0.45 | 2.42 | 6 | 1 |
| 1:A:39:VAL:CG1 | 1:A:74:TYR:CD1 | 0.45 | 3.00 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:63:ARG:HB3 | 1:A:64:PRO:CD | 0.45 | 2.41 | 1 | 2 |
| 1:A:13:VAL:HG11 | 1:A:26:LEU:HD22 | 0.45 | 1.88 | 3 | 1 |
| 1:A:13:VAL:CG1 | 1:A:58:LEU:HD21 | 0.45 | 2.32 | 17 | 1 |
| 1:A:39:VAL:HG21 | 1:A:70:HIS:HB3 | 0.45 | 1.89 | 1 | 1 |
| 1:A:33:TYR:HB3 | 2:B:101:LEU:HD21 | 0.45 | 1.89 | 15 | 1 |
| 2:B:101:LEU:HD13 | 2:B:105:LEU:HD21 | 0.45 | 1.89 | 10 | 1 |
| 1:A:32:MET:O | 1:A:36:THR:N | 0.45 | 2.50 | 13 | 3 |
| 1:A:7:ARG:O | 1:A:11:HIS:CD2 | 0.44 | 2.70 | 2 | 5 |
| 1:A:46:LEU:O | 1:A:50:ILE:N | 0.44 | 2.51 | 17 | 18 |
| 1:A:29:VAL:HG22 | 1:A:45:ASP:CB | 0.44 | 2.43 | 8 | 2 |
| 1:A:33:TYR:CD1 | 1:A:42:LEU:HD22 | 0.44 | 2.48 | 20 | 1 |
| 1:A:35:GLN:HG3 | 1:A:36:THR:HG23 | 0.44 | 1.89 | 7 | 1 |
| 1:A:27:TYR:HA | 1:A:30:LEU:HD12 | 0.44 | 1.90 | 13 | 1 |
| 2:B:101:LEU:O | 2:B:105:LEU:HG | 0.43 | 2.13 | 20 | 2 |
| 1:A:33:TYR:CD2 | 1:A:42:LEU:HD22 | 0.43 | 2.48 | 19 | 2 |
| 1:A:19:ASN:O | 1:A:20:ASP:CB | 0.43 | 2.66 | 3 | 1 |
| 1:A:50:ILE:HG21 | 1:A:59:PHE:HD1 | 0.43 | 1.72 | 10 | 1 |
| 1:A:42:LEU:CD1 | 1:A:46:LEU:CD1 | 0.43 | 2.96 | 20 | 3 |
| 1:A:17:ILE:O | 1:A:17:ILE:CG2 | 0.43 | 2.64 | 9 | 3 |
| 2:B:101:LEU:HG | 2:B:102:LYS:N | 0.43 | 2.29 | 19 | 2 |
| 1:A:16:LEU:O | 1:A:17:ILE:HD13 | 0.43 | 2.14 | 13 | 2 |
| 1:A:33:TYR:CD1 | 1:A:42:LEU:HD12 | 0.42 | 2.49 | 8 | 1 |
| 1:A:46:LEU:HD23 | 1:A:50:ILE:HD12 | 0.42 | 1.91 | 15 | 1 |
| 1:A:49:VAL:HG23 | 1:A:55:ARG:NH2 | 0.42 | 2.29 | 19 | 1 |
| 1:A:13:VAL:O | 1:A:17:ILE:N | 0.42 | 2.52 | 5 | 13 |
| 1:A:61:ALA:O | 1:A:64:PRO:HG2 | 0.42 | 2.15 | 8 | 2 |
| 1:A:23:LYS:O | 1:A:27:TYR:CD2 | 0.42 | 2.73 | 19 | 6 |
| 1:A:26:LEU:HD11 | 1:A:58:LEU:HD22 | 0.42 | 1.92 | 17 | 1 |
| 1:A:7:ARG:O | 1:A:11:HIS:CG | 0.41 | 2.73 | 5 | 2 |
| 1:A:39:VAL:CG2 | 1:A:70:HIS:ND1 | 0.41 | 2.83 | 6 | 2 |
| 1:A:33:TYR:CD1 | 1:A:42:LEU:CD2 | 0.41 | 3.03 | 20 | 1 |
| 1:A:61:ALA:O | 1:A:64:PRO:HD2 | 0.41 | 2.15 | 1 | 1 |
| 1:A:13:VAL:CG1 | 1:A:58:LEU:HD22 | 0.41 | 2.44 | 15 | 2 |
| 1:A:52:GLU:CG | 1:A:55:ARG:CD | 0.41 | 2.98 | 19 | 1 |
| 1:A:23:LYS:O | 1:A:27:TYR:CG | 0.41 | 2.74 | 1 | 2 |
| 1:A:33:TYR:CD2 | 1:A:42:LEU:CD1 | 0.41 | 3.03 | 2 | 1 |
| 1:A:46:LEU:HD13 | 1:A:59:PHE:CD1 | 0.41 | 2.49 | 19 | 1 |
| 1:A:52:GLU:O | 1:A:56:LEU:N | 0.41 | 2.54 | 19 | 5 |
| 1:A:46:LEU:CD1 | 1:A:59:PHE:CE1 | 0.41 | 3.03 | 19 | 1 |
| 1:A:53:PRO:HA | 1:A:56:LEU:HD12 | 0.41 | 1.91 | 4 | 1 |
| 1:A:39:VAL:O | 1:A:43:VAL:CG2 | 0.41 | 2.67 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:TYR:CD1 | 1:A:42:LEU:HD23 | 0.41 | 2.51 | 10 | 1 |
| 1:A:63:ARG:N | 1:A:64:PRO:HD2 | 0.41 | 2.31 | 20 | 1 |
| 1:A:57:PRO:O | 1:A:61:ALA:HB2 | 0.40 | 2.16 | 1 | 1 |
| 1:A:63:ARG:CG | 1:A:74:TYR:CE1 | 0.40 | 3.04 | 4 | 1 |
| 1:A:39:VAL:O | 1:A:39:VAL:HG12 | 0.40 | 2.17 | 2 | 1 |
| 1:A:42:LEU:HD11 | 1:A:74:TYR:HE1 | 0.40 | 1.75 | 9 | 1 |
| 1:A:50:ILE:CG2 | 1:A:56:LEU:HA | 0.40 | 2.46 | 20 | 1 |
| 1:A:46:LEU:CD2 | 1:A:50:ILE:CD1 | 0.40 | 2.99 | 1 | 1 |
| 1:A:67:PRO:O | 1:A:71:GLN:N | 0.40 | 2.54 | 2 | 1 |
| 1:A:63:ARG:O | 1:A:66:ILE:N | 0.40 | 2.55 | 11 | 1 |
| 1:A:23:LYS:O | 1:A:27:TYR:CD1 | 0.40 | 2.75 | 15 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|------------|------------|-------------|-----|
| 1 | A | 72/80 (90%) | 66±1 (91±2%) | 5±2 (8±2%) | 1±1 (1±1%) | 14 | 59 |
| 2 | B | 8/16 (50%) | 8±0 (97±5%) | 0±0 (3±5%) | 0±0 (0±0%) | 100 | 100 |
| All | All | 1600/1920 (83%) | 1466 (92%) | 113 (7%) | 21 (1%) | 16 | 63 |

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 17 | ILE | 13 |
| 1 | A | 64 | PRO | 6 |
| 1 | A | 3 | ARG | 2 |

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 | 67/75 (89%) | 51±3 (76±4%) | 16±3 (24±4%) | 2 | 26 |
| 2 | B | 8/15 (53%) | 6±1 (69±10%) | 2±1 (31±10%) | 1 | 14 |
| All | All | 1500/1800 (83%) | 1126 (75%) | 374 (25%) | 2 | 25 |

All 48 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 | 9 | PHE | 20 |
| 1 | A | 62 | ILE | 20 |
| 1 | A | 59 | PHE | 19 |
| 1 | A | 66 | ILE | 15 |
| 1 | A | 25 | TYR | 14 |
| 1 | A | 10 | ARG | 13 |
| 1 | A | 47 | LYS | 13 |
| 1 | A | 71 | GLN | 13 |
| 2 | B | 105 | LEU | 13 |
| 2 | B | 103 | GLU | 13 |
| 1 | A | 7 | ARG | 12 |
| 1 | A | 3 | ARG | 12 |
| 1 | A | 69 | LYS | 11 |
| 1 | A | 4 | LYS | 11 |
| 1 | A | 26 | LEU | 10 |
| 1 | A | 31 | ARG | 10 |
| 2 | B | 102 | LYS | 10 |
| 1 | A | 35 | GLN | 10 |
| 1 | A | 32 | MET | 10 |
| 1 | A | 42 | LEU | 9 |
| 1 | A | 38 | ASP | 8 |
| 1 | A | 60 | ASP | 7 |
| 1 | A | 63 | ARG | 7 |
| 1 | A | 24 | ASP | 7 |
| 1 | A | 54 | SER | 7 |
| 2 | B | 101 | LEU | 7 |
| 1 | A | 48 | LEU | 6 |
| 1 | A | 28 | ASP | 6 |
| 1 | A | 19 | ASN | 5 |
| 1 | A | 20 | ASP | 5 |
| 1 | A | 73 | GLU | 5 |
| 1 | A | 34 | HIS | 5 |
| 2 | B | 106 | GLU | 5 |
| 1 | A | 55 | ARG | 4 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 33 | TYR | 4 |
| 1 | A | 45 | ASP | 4 |
| 1 | A | 18 | GLU | 3 |
| 1 | A | 36 | THR | 3 |
| 1 | A | 68 | LEU | 3 |
| 1 | A | 8 | GLU | 3 |
| 1 | A | 23 | LYS | 2 |
| 1 | A | 46 | LEU | 2 |
| 2 | B | 100 | LEU | 2 |
| 1 | A | 12 | LYS | 2 |
| 1 | A | 58 | LEU | 1 |
| 1 | A | 51 | ASN | 1 |
| 1 | A | 37 | MET | 1 |
| 1 | A | 52 | 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](#)

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 78% 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 | 1132 |
| Number of shifts mapped to atoms | 1132 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 93 | -1.21 \pm 0.28 | Should be checked |
| $^{13}\text{C}_\beta$ | 91 | -0.54 \pm 0.08 | Should be checked |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 86 | -0.17 \pm 0.27 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 978 atoms were assigned a chemical shift out of a possible 1206. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 313/393 (80%) | 157/157 (100%) | 80/160 (50%) | 76/76 (100%) |
| Sidechain | 632/723 (87%) | 432/470 (92%) | 196/225 (87%) | 4/28 (14%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 33/90 (37%) | 33/43 (77%) | 0/41 (0%) | 0/6 (0%) |
| Overall | 978/1206 (81%) | 622/670 (93%) | 276/426 (65%) | 80/110 (73%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1131 atoms were assigned a chemical shift out of a possible 1444. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 359/472 (76%) | 180/189 (95%) | 93/192 (48%) | 86/91 (95%) |
| Sidechain | 735/873 (84%) | 501/566 (89%) | 229/270 (85%) | 5/37 (14%) |
| Aromatic | 37/99 (37%) | 37/47 (79%) | 0/46 (0%) | 0/6 (0%) |
| Overall | 1131/1444 (78%) | 718/802 (90%) | 322/508 (63%) | 91/134 (68%) |

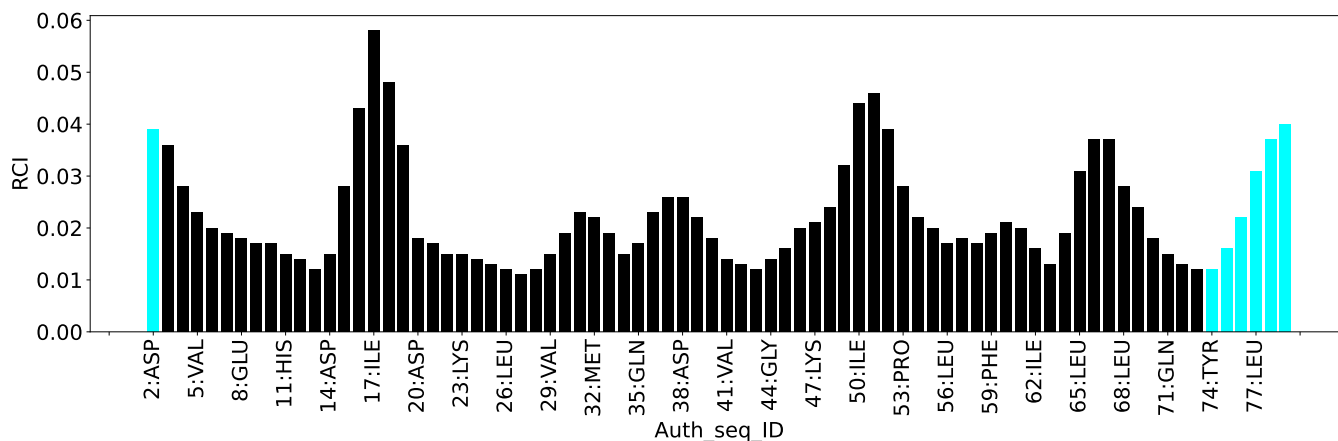
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

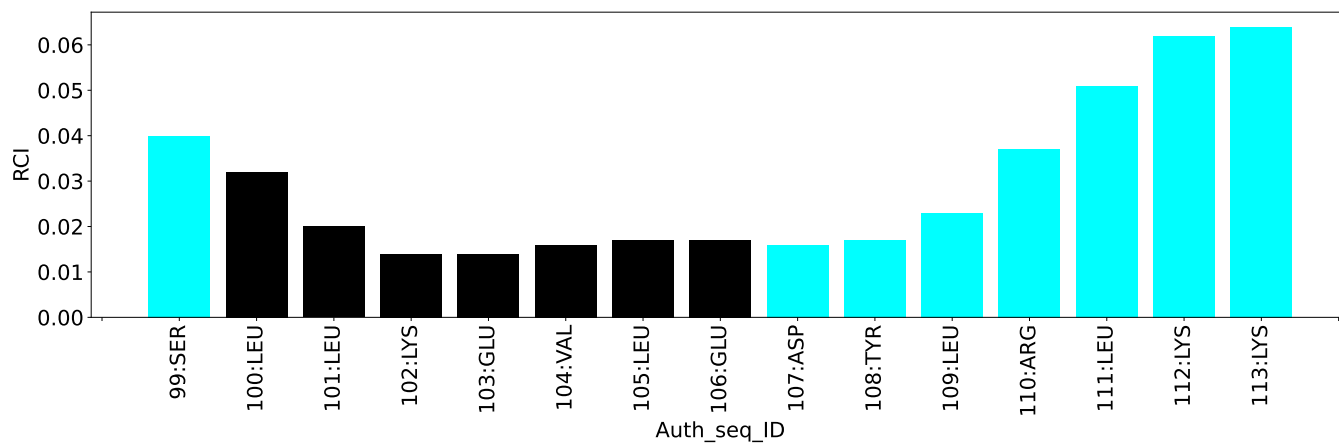
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 1781 |
| Intra-residue ($ i-j =0$) | 670 |
| Sequential ($ i-j =1$) | 386 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 360 |
| Long range ($ i-j \geq 5$) | 210 |
| Inter-chain | 67 |
| Hydrogen bond restraints | 88 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 138 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 20.0 |
| Number of long range restraints per residue ¹ | 2.2 |

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

| Bins (Å) | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small) | 5.5 | 0.2 |
| 0.2-0.5 (Medium) | 0.6 | 0.29 |
| >0.5 (Large) | None | None |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 0.3 | 1.4 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis i

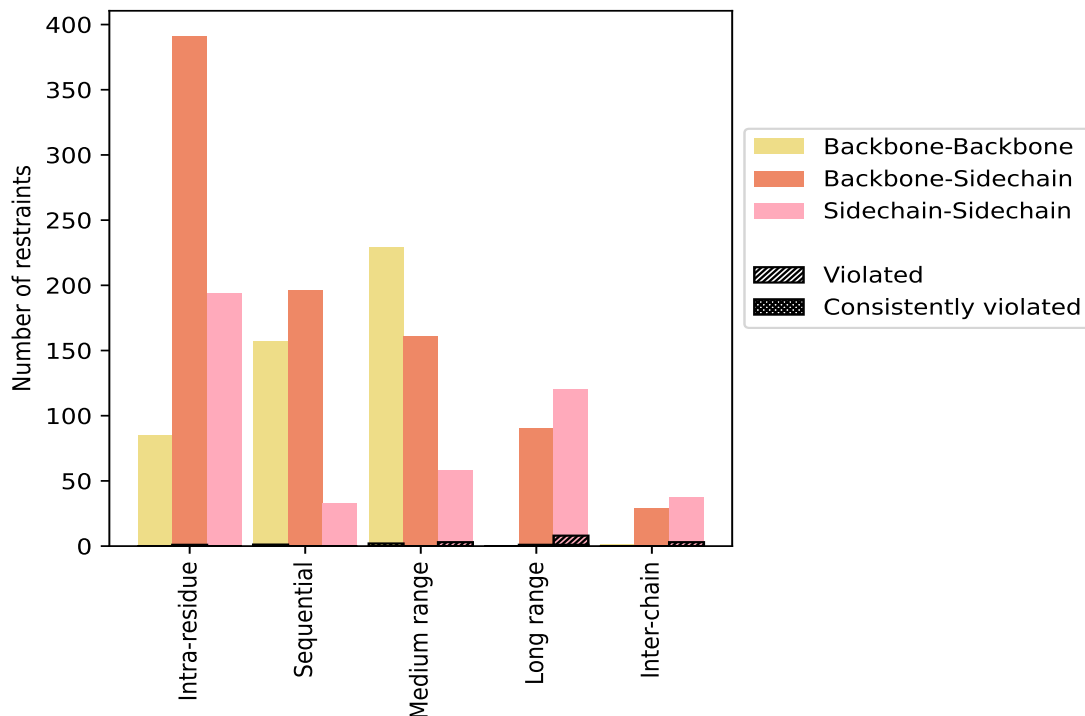
9.1 Summary of distance violations i

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.

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 670 | 37.6 | 1 | 0.1 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 85 | 4.8 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 391 | 22.0 | 1 | 0.3 | 0.1 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 194 | 10.9 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sequential ($i-j =1$) | 386 | 21.7 | 1 | 0.3 | 0.1 | 1 | 0.3 | 0.1 |
| Backbone-Backbone | 157 | 8.8 | 1 | 0.6 | 0.1 | 1 | 0.6 | 0.1 |
| Backbone-Sidechain | 196 | 11.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 33 | 1.9 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Medium range ($i-j >1$ & $i-j <5$) | 360 | 20.2 | 5 | 1.4 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 141 | 7.9 | 2 | 1.4 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 161 | 9.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 58 | 3.3 | 3 | 5.2 | 0.2 | 0 | 0.0 | 0.0 |
| Long range ($i-j \geq 5$) | 210 | 11.8 | 9 | 4.3 | 0.5 | 1 | 0.5 | 0.1 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 90 | 5.1 | 1 | 1.1 | 0.1 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 120 | 6.7 | 8 | 6.7 | 0.4 | 1 | 0.8 | 0.1 |
| Inter-chain | 67 | 3.8 | 3 | 4.5 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 1 | 0.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 29 | 1.6 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 37 | 2.1 | 3 | 8.1 | 0.2 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 88 | 4.9 | 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 | 1781 | 100.0 | 19 | 1.1 | 1.1 | 2 | 0.1 | 0.1 |
| Backbone-Backbone | 472 | 26.5 | 3 | 0.6 | 0.2 | 1 | 0.2 | 0.1 |
| Backbone-Sidechain | 867 | 48.7 | 2 | 0.2 | 0.1 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 442 | 24.8 | 14 | 3.2 | 0.8 | 1 | 0.2 | 0.1 |

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 disulfid 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 | 0 | 1 | 2 | 4 | 1 | 8 | 0.14 | 0.24 | 0.04 | 0.12 |
| 2 | 0 | 1 | 0 | 2 | 1 | 4 | 0.13 | 0.18 | 0.03 | 0.12 |
| 3 | 0 | 1 | 0 | 2 | 1 | 4 | 0.18 | 0.25 | 0.05 | 0.18 |
| 4 | 0 | 1 | 2 | 2 | 2 | 7 | 0.15 | 0.25 | 0.05 | 0.13 |
| 5 | 0 | 1 | 1 | 2 | 1 | 5 | 0.13 | 0.18 | 0.02 | 0.13 |
| 6 | 0 | 1 | 2 | 4 | 1 | 8 | 0.15 | 0.19 | 0.02 | 0.15 |
| 7 | 0 | 1 | 1 | 1 | 2 | 5 | 0.15 | 0.24 | 0.05 | 0.13 |
| 8 | 0 | 1 | 0 | 5 | 2 | 8 | 0.15 | 0.29 | 0.05 | 0.14 |
| 9 | 0 | 1 | 1 | 3 | 0 | 5 | 0.14 | 0.22 | 0.04 | 0.12 |
| 10 | 0 | 1 | 1 | 1 | 1 | 4 | 0.16 | 0.2 | 0.03 | 0.16 |
| 11 | 0 | 1 | 0 | 4 | 2 | 7 | 0.14 | 0.19 | 0.03 | 0.14 |

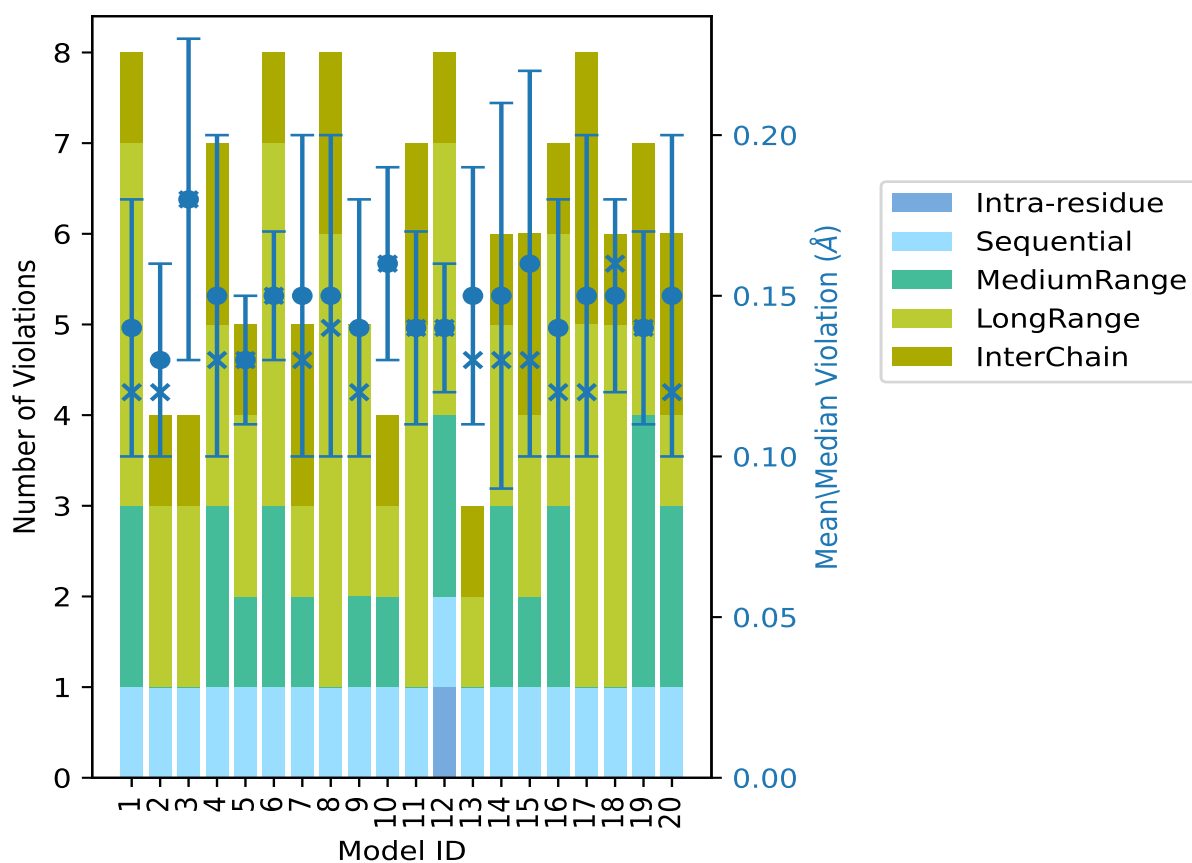
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 12 | 1 | 1 | 2 | 3 | 1 | 8 | 0.14 | 0.19 | 0.02 | 0.14 |
| 13 | 0 | 1 | 0 | 1 | 1 | 3 | 0.15 | 0.2 | 0.04 | 0.13 |
| 14 | 0 | 1 | 2 | 2 | 1 | 6 | 0.15 | 0.29 | 0.06 | 0.13 |
| 15 | 0 | 1 | 1 | 2 | 2 | 6 | 0.16 | 0.29 | 0.06 | 0.13 |
| 16 | 0 | 1 | 2 | 3 | 1 | 7 | 0.14 | 0.24 | 0.04 | 0.12 |
| 17 | 0 | 1 | 0 | 4 | 3 | 8 | 0.15 | 0.26 | 0.05 | 0.12 |
| 18 | 0 | 1 | 0 | 4 | 1 | 6 | 0.15 | 0.19 | 0.03 | 0.16 |
| 19 | 0 | 1 | 3 | 1 | 2 | 7 | 0.14 | 0.19 | 0.03 | 0.14 |
| 20 | 0 | 1 | 2 | 1 | 2 | 6 | 0.15 | 0.25 | 0.05 | 0.12 |

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

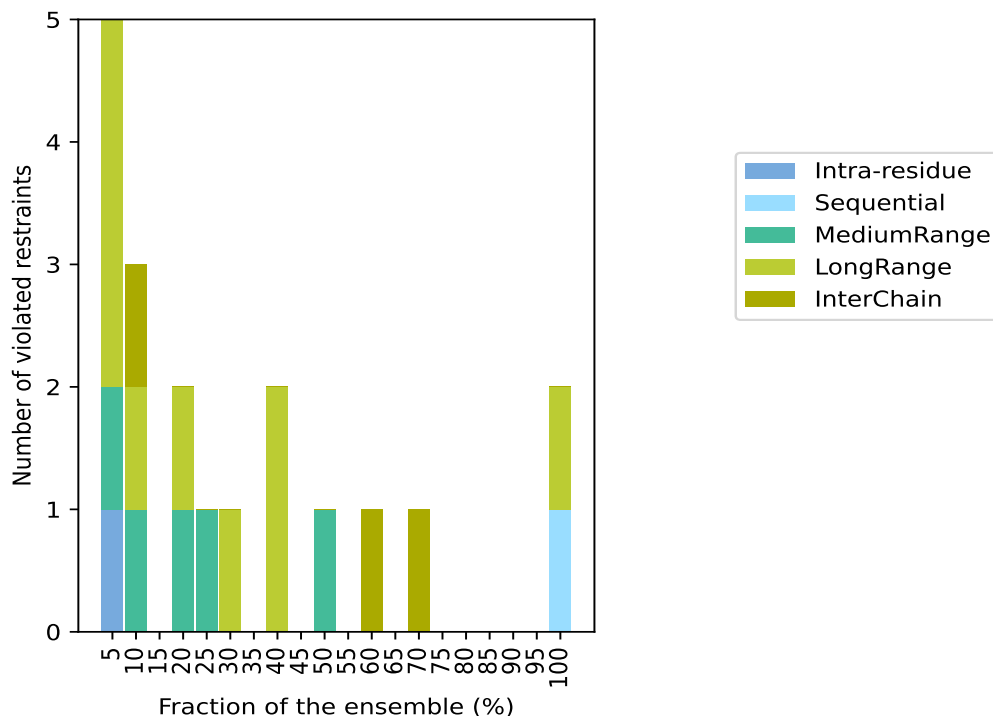
9.3 Distance violation statistics for the ensemble

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, 1674(IR:669, SQ:385, MR:355, LR:201, IC:64) restraints are not violated in the ensemble.

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

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

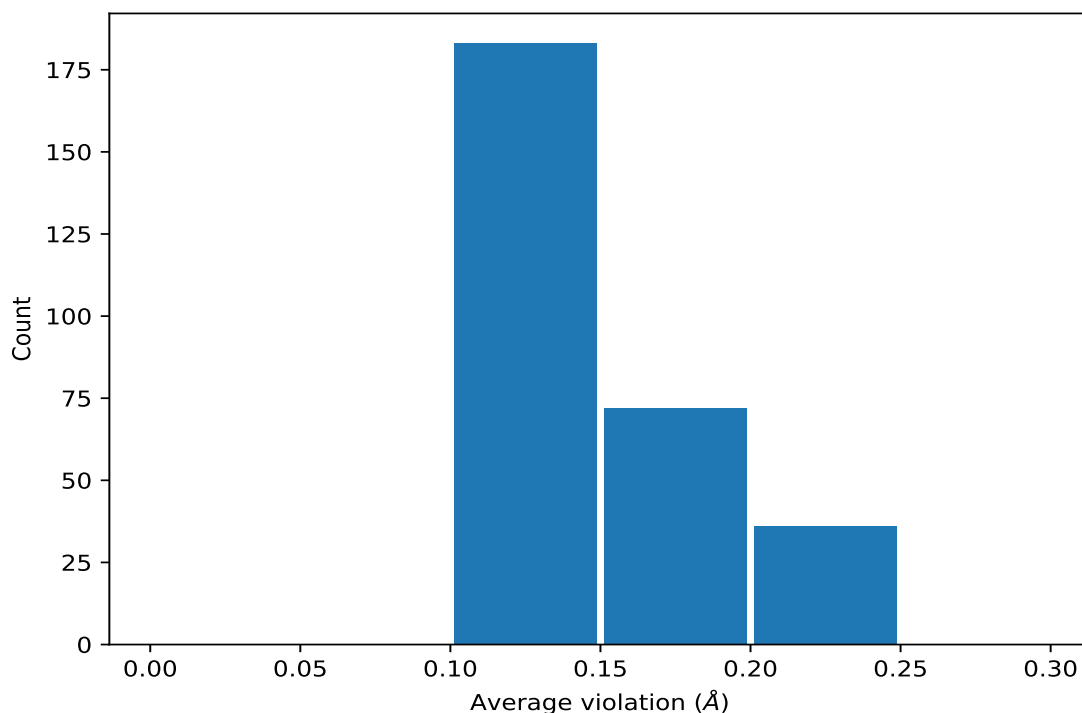
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 20 | 0.22 | 0.05 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 20 | 0.22 | 0.05 | 0.21 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 20 | 0.22 | 0.05 | 0.21 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 20 | 0.12 | 0.01 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 14 | 0.17 | 0.04 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 14 | 0.17 | 0.04 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 14 | 0.17 | 0.04 | 0.18 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 12 | 0.13 | 0.01 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 12 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 10 | 0.13 | 0.01 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 10 | 0.13 | 0.01 | 0.13 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 8 | 0.14 | 0.02 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 8 | 0.14 | 0.02 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 8 | 0.14 | 0.02 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD11 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD12 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD13 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD21 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD22 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD23 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD11 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD12 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD13 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD21 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD22 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD23 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD11 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD12 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD13 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD21 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD22 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD23 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD11 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD12 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD13 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD21 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD22 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD23 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD11 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD12 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD13 | 6 | 0.15 | 0.01 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD21 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD22 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD23 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD11 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD12 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD13 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD21 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD22 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD23 | 6 | 0.15 | 0.01 | 0.15 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD11 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD12 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD13 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD11 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD12 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD13 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD11 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD12 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD13 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD11 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD12 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD13 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD11 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD12 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD13 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD11 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD12 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD13 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB2 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB3 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB2 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB3 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB2 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB3 | 4 | 0.12 | 0.0 | 0.12 |
| (1,532) | 1:A:52:GLU:H | 1:A:55:ARG:HA | 4 | 0.11 | 0.0 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG11 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG12 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG13 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG21 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG22 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG23 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG11 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG12 | 2 | 0.14 | 0.02 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG13 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG21 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG22 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG23 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG11 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG12 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG13 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG21 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG22 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG23 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG11 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG12 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG13 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG21 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG22 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG23 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG11 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG12 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG13 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG21 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG22 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG23 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG11 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG12 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG13 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG21 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG22 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG23 | 2 | 0.14 | 0.02 | 0.14 |
| (1,853) | 2:B:110:ARG:HA | 2:B:112:LYS:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD11 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD13 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD11 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD13 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD11 | 2 | 0.12 | 0.0 | 0.12 |

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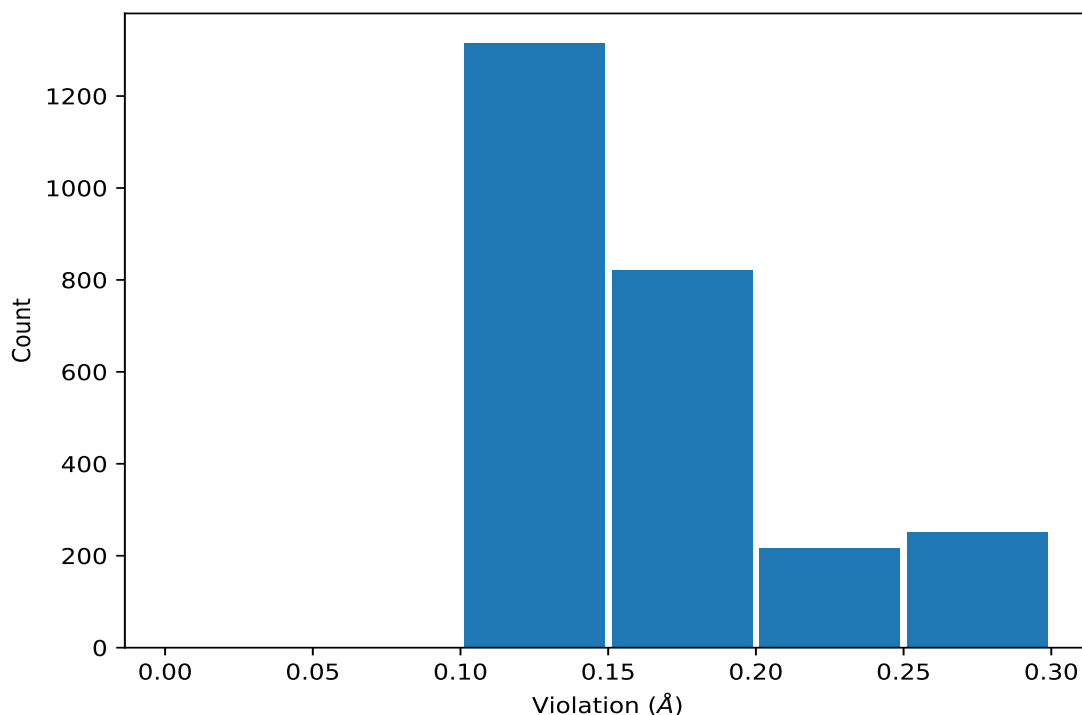
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD13 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD11 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD13 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD11 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD13 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD11 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD13 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |

¹Number of violated models, ²Standard 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) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 8 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 8 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 14 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 14 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 15 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 15 | 0.29 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 17 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 17 | 0.26 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 3 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 20 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 20 | 0.25 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 20 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 4 | 0.25 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 4 | 0.25 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 1 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 1 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 7 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 7 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 16 | 0.24 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 16 | 0.24 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 9 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 9 | 0.22 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 13 | 0.2 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 13 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 10 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 10 | 0.2 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 10 | 0.2 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 4 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 4 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 6 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 6 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 11 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 11 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 18 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 18 | 0.19 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 18 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 3 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 3 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 12 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 19 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 19 | 0.19 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 19 | 0.19 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 2 | 0.18 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 2 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 5 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 5 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 10 | 0.18 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 10 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 1 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 1 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 17 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 20 | 0.18 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 20 | 0.18 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 19 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 19 | 0.17 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 19 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 11 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 11 | 0.17 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 11 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 18 | 0.17 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 18 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD11 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD12 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD13 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD21 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD22 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD23 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD11 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD12 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD13 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD21 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD22 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD23 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD11 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD12 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD13 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD21 | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD22 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD23 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD11 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD12 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD13 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD21 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD22 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD23 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD11 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD12 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD13 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD21 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD22 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD23 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD11 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD12 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD13 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD21 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD22 | 3 | 0.17 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD23 | 3 | 0.17 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 8 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 11 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 11 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 18 | 0.16 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD11 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD12 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD13 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD21 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD22 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD23 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD11 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD12 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD13 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD21 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD22 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD23 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD11 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD12 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD13 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD21 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD22 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD23 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD11 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD12 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD13 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD21 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD22 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD23 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD11 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD12 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD13 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD21 | 18 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD22 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD23 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD11 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD12 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD13 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD21 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD22 | 18 | 0.16 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD23 | 18 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG11 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG12 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG13 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG21 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG22 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG23 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG11 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG12 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG13 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG21 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG22 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG23 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG11 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG12 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG13 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG21 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG22 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG23 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG11 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG12 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG13 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG21 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG22 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG23 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG11 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG12 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG13 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG21 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG22 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG23 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG11 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG12 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG13 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG21 | 15 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG22 | 15 | 0.16 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG23 | 15 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD11 | 1:A:58:LEU:HD11 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD11 | 1:A:58:LEU:HD12 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD11 | 1:A:58:LEU:HD13 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD11 | 1:A:58:LEU:HD21 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD11 | 1:A:58:LEU:HD22 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD11 | 1:A:58:LEU:HD23 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD12 | 1:A:58:LEU:HD11 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD12 | 1:A:58:LEU:HD12 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD12 | 1:A:58:LEU:HD13 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD12 | 1:A:58:LEU:HD21 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD12 | 1:A:58:LEU:HD22 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD12 | 1:A:58:LEU:HD23 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD13 | 1:A:58:LEU:HD11 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD13 | 1:A:58:LEU:HD12 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD13 | 1:A:58:LEU:HD13 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD13 | 1:A:58:LEU:HD21 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD13 | 1:A:58:LEU:HD22 | 6 | 0.16 |
| (1,1019) | 1:A:17:ILE:HD13 | 1:A:58:LEU:HD23 | 6 | 0.16 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 4 | 0.15 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 4 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 6 | 0.15 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 6 | 0.15 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 6 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 17 | 0.15 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 17 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD11 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD12 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD13 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD21 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD22 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD23 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD11 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD12 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD13 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD21 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD22 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD23 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD11 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD12 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD13 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD21 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD22 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD23 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD11 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD12 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD13 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD21 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD22 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD23 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD11 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD12 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD13 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD21 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD22 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD23 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD11 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD12 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD13 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD21 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD22 | 8 | 0.15 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD23 | 8 | 0.15 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 12 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD11 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD12 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD13 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD21 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD22 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG11 | 1:A:58:LEU:HD23 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD11 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD12 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD13 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD21 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD22 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG12 | 1:A:58:LEU:HD23 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD11 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD12 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD13 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD21 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD22 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG13 | 1:A:58:LEU:HD23 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD11 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD12 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD13 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD21 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD22 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG21 | 1:A:58:LEU:HD23 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD11 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD12 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD13 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD21 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD22 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG22 | 1:A:58:LEU:HD23 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD11 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD12 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD13 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD21 | 19 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD22 | 19 | 0.14 |
| (1,977) | 1:A:13:VAL:HG23 | 1:A:58:LEU:HD23 | 19 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 8 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 14 | 0.14 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 14 | 0.14 |
| (1,869) | 2:B:112:LYS:HG2 | 2:B:112:LYS:H | 12 | 0.14 |
| (1,869) | 2:B:112:LYS:HG3 | 2:B:112:LYS:H | 12 | 0.14 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD11 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD12 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD13 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD11 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD12 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD13 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD11 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD12 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD13 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD11 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD12 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD13 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD11 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD12 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD13 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD11 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD12 | 6 | 0.14 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD13 | 6 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 12 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 14 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 14 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 19 | 0.14 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 19 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 12 | 0.14 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 12 | 0.14 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 12 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD11 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD12 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD13 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD21 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD22 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD23 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD11 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD12 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD13 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD21 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD22 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD23 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD11 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD12 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD13 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD21 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD22 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD23 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD11 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD12 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD13 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD21 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD22 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD23 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD11 | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD12 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD13 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD21 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD22 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD23 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD11 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD12 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD13 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD21 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD22 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD23 | 1 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD11 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD12 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD13 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD21 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD22 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD23 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD11 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD12 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD13 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD21 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD22 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD23 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD11 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD12 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD13 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD21 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD22 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD23 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD11 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD12 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD13 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD21 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD22 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD23 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD11 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD12 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD13 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD21 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD22 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD23 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD11 | 11 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD12 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD13 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD21 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD22 | 11 | 0.14 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD23 | 11 | 0.14 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 5 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 7 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 11 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|---------------|------------------|----------|---------------|
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 11 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 13 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 15 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 15 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 16 | 0.13 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 16 | 0.13 |
| (1,853) | 2:B:110:ARG:HA | 2:B:112:LYS:H | 16 | 0.13 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 10 | 0.13 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 15 | 0.13 |
| (1,1280) | 1:A:50:ILE:HA | 1:A:55:ARG:HB2 | 8 | 0.13 |
| (1,1280) | 1:A:50:ILE:HA | 1:A:55:ARG:HB3 | 8 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD11 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD12 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD13 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD11 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD12 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD13 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD11 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD12 | 19 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD13 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD11 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD12 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD13 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD11 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD12 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD13 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD11 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD12 | 19 | 0.13 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD13 | 19 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 4 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 7 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 10 | 0.13 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 10 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 1 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 1 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 5 | 0.13 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 5 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD11 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD12 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD13 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD21 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD22 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG11 | 1:A:42:LEU:HD23 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD11 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD12 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD13 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD21 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD22 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG12 | 1:A:42:LEU:HD23 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD11 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD12 | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD13 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD21 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD22 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG13 | 1:A:42:LEU:HD23 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD11 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD12 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD13 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD21 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD22 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG21 | 1:A:42:LEU:HD23 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD11 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD12 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD13 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD21 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD22 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG22 | 1:A:42:LEU:HD23 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD11 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD12 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD13 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD21 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD22 | 17 | 0.13 |
| (1,1098) | 1:A:29:VAL:HG23 | 1:A:42:LEU:HD23 | 17 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD11 | 1:A:58:LEU:HD11 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD11 | 1:A:58:LEU:HD12 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD11 | 1:A:58:LEU:HD13 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD11 | 1:A:58:LEU:HD21 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD11 | 1:A:58:LEU:HD22 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD11 | 1:A:58:LEU:HD23 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD12 | 1:A:58:LEU:HD11 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD12 | 1:A:58:LEU:HD12 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD12 | 1:A:58:LEU:HD13 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD12 | 1:A:58:LEU:HD21 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD12 | 1:A:58:LEU:HD22 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD12 | 1:A:58:LEU:HD23 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD13 | 1:A:58:LEU:HD11 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD13 | 1:A:58:LEU:HD12 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD13 | 1:A:58:LEU:HD13 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD13 | 1:A:58:LEU:HD21 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD13 | 1:A:58:LEU:HD22 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD13 | 1:A:58:LEU:HD23 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD21 | 1:A:58:LEU:HD11 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD21 | 1:A:58:LEU:HD12 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1080) | 1:A:26:LEU:HD21 | 1:A:58:LEU:HD13 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD21 | 1:A:58:LEU:HD21 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD21 | 1:A:58:LEU:HD22 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD21 | 1:A:58:LEU:HD23 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD22 | 1:A:58:LEU:HD11 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD22 | 1:A:58:LEU:HD12 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD22 | 1:A:58:LEU:HD13 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD22 | 1:A:58:LEU:HD21 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD22 | 1:A:58:LEU:HD22 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD22 | 1:A:58:LEU:HD23 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD23 | 1:A:58:LEU:HD11 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD23 | 1:A:58:LEU:HD12 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD23 | 1:A:58:LEU:HD13 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD23 | 1:A:58:LEU:HD21 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD23 | 1:A:58:LEU:HD22 | 9 | 0.13 |
| (1,1080) | 1:A:26:LEU:HD23 | 1:A:58:LEU:HD23 | 9 | 0.13 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 17 | 0.12 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 17 | 0.12 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 3 | 0.12 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 7 | 0.12 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 8 | 0.12 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 9 | 0.12 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 12 | 0.12 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 16 | 0.12 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 17 | 0.12 |
| (1,1428) | 1:A:66:ILE:HG21 | 1:A:70:HIS:HB2 | 16 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1428) | 1:A:66:ILE:HG21 | 1:A:70:HIS:HB3 | 16 | 0.12 |
| (1,1428) | 1:A:66:ILE:HG22 | 1:A:70:HIS:HB2 | 16 | 0.12 |
| (1,1428) | 1:A:66:ILE:HG22 | 1:A:70:HIS:HB3 | 16 | 0.12 |
| (1,1428) | 1:A:66:ILE:HG23 | 1:A:70:HIS:HB2 | 16 | 0.12 |
| (1,1428) | 1:A:66:ILE:HG23 | 1:A:70:HIS:HB3 | 16 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 2 | 0.12 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 2 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD11 | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD12 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD13 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD11 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD12 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD13 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD11 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD12 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD13 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD11 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD12 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD13 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD11 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD12 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD13 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD11 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD12 | 15 | 0.12 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD13 | 15 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 5 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 6 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 9 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD11 | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD12 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD13 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD21 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD22 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD11 | 1:A:46:LEU:HD23 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD11 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD12 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD13 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD21 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD22 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD12 | 1:A:46:LEU:HD23 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD11 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD12 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD13 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD21 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD22 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD13 | 1:A:46:LEU:HD23 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD11 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD12 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD13 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD21 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD22 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD21 | 1:A:46:LEU:HD23 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD11 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD12 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD13 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD21 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD22 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD22 | 1:A:46:LEU:HD23 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD11 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD12 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD13 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD21 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD22 | 20 | 0.12 |
| (1,1212) | 1:A:42:LEU:HD23 | 1:A:46:LEU:HD23 | 20 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 4 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 14 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD11 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD12 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD11 | 1:A:62:ILE:HD13 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD11 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD12 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD12 | 1:A:62:ILE:HD13 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD11 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD12 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD13 | 1:A:62:ILE:HD13 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD11 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD12 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD21 | 1:A:62:ILE:HD13 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD11 | 16 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD12 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD22 | 1:A:62:ILE:HD13 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD11 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD12 | 16 | 0.12 |
| (1,1119) | 1:A:30:LEU:HD23 | 1:A:62:ILE:HD13 | 16 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD11 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD12 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD13 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD21 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD22 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD23 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD11 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD12 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD13 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD21 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD22 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD23 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD11 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD12 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD13 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD21 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD22 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD23 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD11 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD12 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD13 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD21 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD22 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD23 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD11 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD12 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD13 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD21 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD22 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD23 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD11 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD12 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD13 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD21 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD22 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD23 | 17 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD11 | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD12 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD13 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD21 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD22 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD11 | 2:B:101:LEU:HD23 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD11 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD12 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD13 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD21 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD22 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD12 | 2:B:101:LEU:HD23 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD11 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD12 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD13 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD21 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD22 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD13 | 2:B:101:LEU:HD23 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD11 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD12 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD13 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD21 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD22 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD21 | 2:B:101:LEU:HD23 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD11 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD12 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD13 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD21 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD22 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD22 | 2:B:101:LEU:HD23 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD11 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD12 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD13 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD21 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD22 | 20 | 0.12 |
| (1,1114) | 1:A:30:LEU:HD23 | 2:B:101:LEU:HD23 | 20 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 12 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 12 | 0.12 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 12 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB2 | 8 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB3 | 8 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB2 | 8 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB3 | 8 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB2 | 8 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB3 | 8 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB2 | 9 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB3 | 9 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB2 | 9 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB3 | 9 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB2 | 9 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB3 | 9 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB2 | 16 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB3 | 16 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB2 | 16 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB3 | 16 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB2 | 16 | 0.12 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB3 | 16 | 0.12 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG11 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG12 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG13 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG21 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG22 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB1 | 2:B:104:VAL:HG23 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG11 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG12 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG13 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG21 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG22 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB2 | 2:B:104:VAL:HG23 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG11 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG12 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG13 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG21 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG22 | 18 | 0.11 |
| (1,916) | 1:A:6:ALA:HB3 | 2:B:104:VAL:HG23 | 18 | 0.11 |
| (1,853) | 2:B:110:ARG:HA | 2:B:112:LYS:H | 12 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,532) | 1:A:52:GLU:H | 1:A:55:ARG:HA | 1 | 0.11 |
| (1,532) | 1:A:52:GLU:H | 1:A:55:ARG:HA | 4 | 0.11 |
| (1,532) | 1:A:52:GLU:H | 1:A:55:ARG:HA | 19 | 0.11 |
| (1,532) | 1:A:52:GLU:H | 1:A:55:ARG:HA | 20 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 1 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 2 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 4 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 5 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 11 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 13 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 14 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 18 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 19 | 0.11 |
| (1,160) | 1:A:17:ILE:H | 1:A:18:GLU:H | 20 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 7 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 8 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG11 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG12 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG13 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG21 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG22 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD11 | 2:B:104:VAL:HG23 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG11 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG12 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG13 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG21 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG22 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD12 | 2:B:104:VAL:HG23 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG11 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG12 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG13 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG21 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG22 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD13 | 2:B:104:VAL:HG23 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG11 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG12 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG13 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG21 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG22 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD21 | 2:B:104:VAL:HG23 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG11 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG12 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG13 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG21 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG22 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD22 | 2:B:104:VAL:HG23 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG11 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG12 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG13 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG21 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG22 | 15 | 0.11 |
| (1,1406) | 1:A:65:LEU:HD23 | 2:B:104:VAL:HG23 | 15 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD11 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD12 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD13 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD11 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD12 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD13 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD11 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD12 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD13 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD11 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD12 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD13 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD11 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD12 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD13 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD11 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD12 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD13 | 1 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD11 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD12 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD11 | 1:A:50:ILE:HD13 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD11 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD12 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD12 | 1:A:50:ILE:HD13 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD11 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD12 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD13 | 1:A:50:ILE:HD13 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD11 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD12 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD21 | 1:A:50:ILE:HD13 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD11 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD12 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD22 | 1:A:50:ILE:HD13 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD11 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD12 | 14 | 0.11 |
| (1,1249) | 1:A:46:LEU:HD23 | 1:A:50:ILE:HD13 | 14 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 1 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 2 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB2 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG11 | 1:A:45:ASP:HB3 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB2 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG12 | 1:A:45:ASP:HB3 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB2 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG13 | 1:A:45:ASP:HB3 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB2 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG21 | 1:A:45:ASP:HB3 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB2 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG22 | 1:A:45:ASP:HB3 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB2 | 6 | 0.11 |
| (1,1100) | 1:A:29:VAL:HG23 | 1:A:45:ASP:HB3 | 6 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG11 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG12 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG13 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG21 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG22 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD11 | 1:A:49:VAL:HG23 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG11 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG12 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG13 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG21 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG22 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD12 | 1:A:49:VAL:HG23 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG11 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG12 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG13 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG21 | 11 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG22 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD13 | 1:A:49:VAL:HG23 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG11 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG12 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG13 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG21 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG22 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD21 | 1:A:49:VAL:HG23 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG11 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG12 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG13 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG21 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG22 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD22 | 1:A:49:VAL:HG23 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG11 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG12 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG13 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG21 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG22 | 11 | 0.11 |
| (1,1078) | 1:A:26:LEU:HD23 | 1:A:49:VAL:HG23 | 11 | 0.11 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB2 | 17 | 0.11 |
| (1,1023) | 1:A:17:ILE:HG21 | 1:A:22:GLU:HB3 | 17 | 0.11 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB2 | 17 | 0.11 |
| (1,1023) | 1:A:17:ILE:HG22 | 1:A:22:GLU:HB3 | 17 | 0.11 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB2 | 17 | 0.11 |
| (1,1023) | 1:A:17:ILE:HG23 | 1:A:22:GLU:HB3 | 17 | 0.11 |

10 Dihedral-angle violation analysis [i](#)

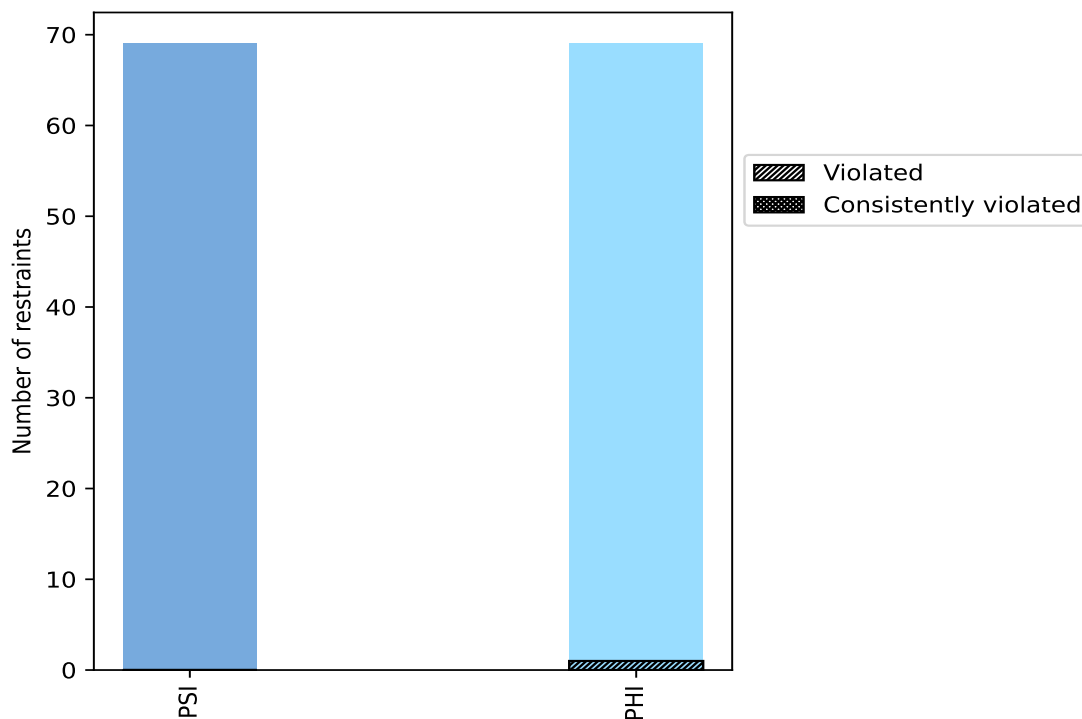
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PSI | 69 | 50.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| PHI | 69 | 50.0 | 1 | 1.4 | 0.7 | 0 | 0.0 | 0.0 |
| Total | 138 | 100.0 | 1 | 0.7 | 0.7 | 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](#)



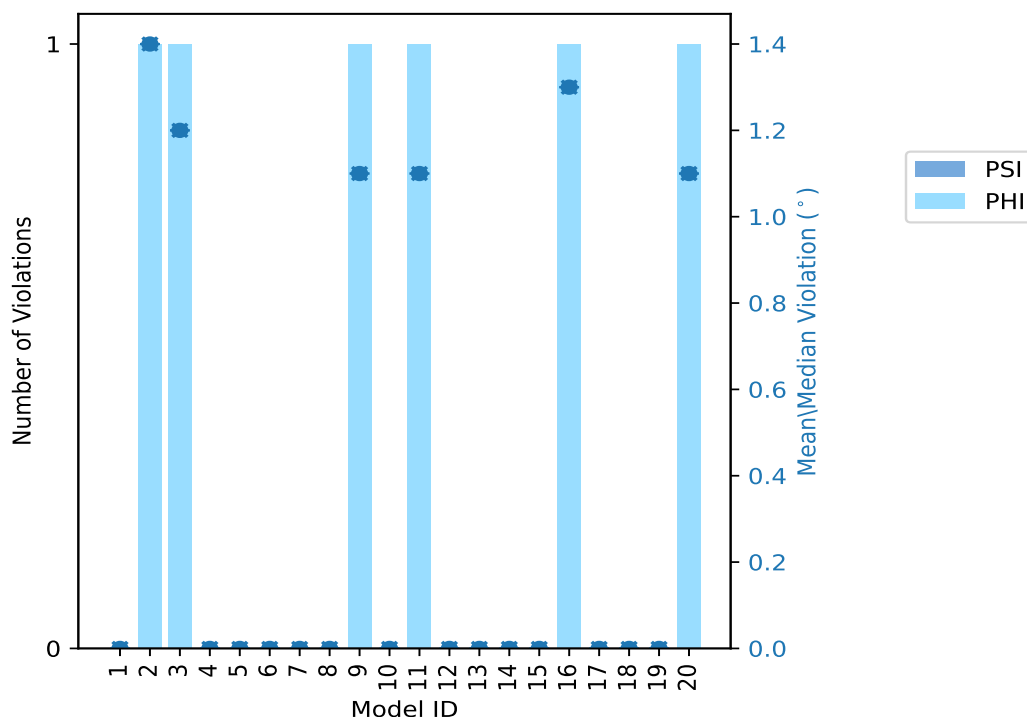
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 2 | 0 | 1 | 1 | 1.4 | 1.4 | 0.0 | 1.4 |
| 3 | 0 | 1 | 1 | 1.2 | 1.2 | 0.0 | 1.2 |
| 4 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 5 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 6 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 7 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 8 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 9 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 10 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 11 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 12 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 14 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 15 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 16 | 0 | 1 | 1 | 1.3 | 1.3 | 0.0 | 1.3 |
| 17 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 18 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 19 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 20 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |

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 | % |
| 0 | 0 | 0 | 1 | 5.0 |
| 0 | 0 | 0 | 2 | 10.0 |
| 0 | 0 | 0 | 3 | 15.0 |
| 0 | 0 | 0 | 4 | 20.0 |
| 0 | 0 | 0 | 5 | 25.0 |
| 0 | 1 | 1 | 6 | 30.0 |
| 0 | 0 | 0 | 7 | 35.0 |
| 0 | 0 | 0 | 8 | 40.0 |
| 0 | 0 | 0 | 9 | 45.0 |
| 0 | 0 | 0 | 10 | 50.0 |
| 0 | 0 | 0 | 11 | 55.0 |

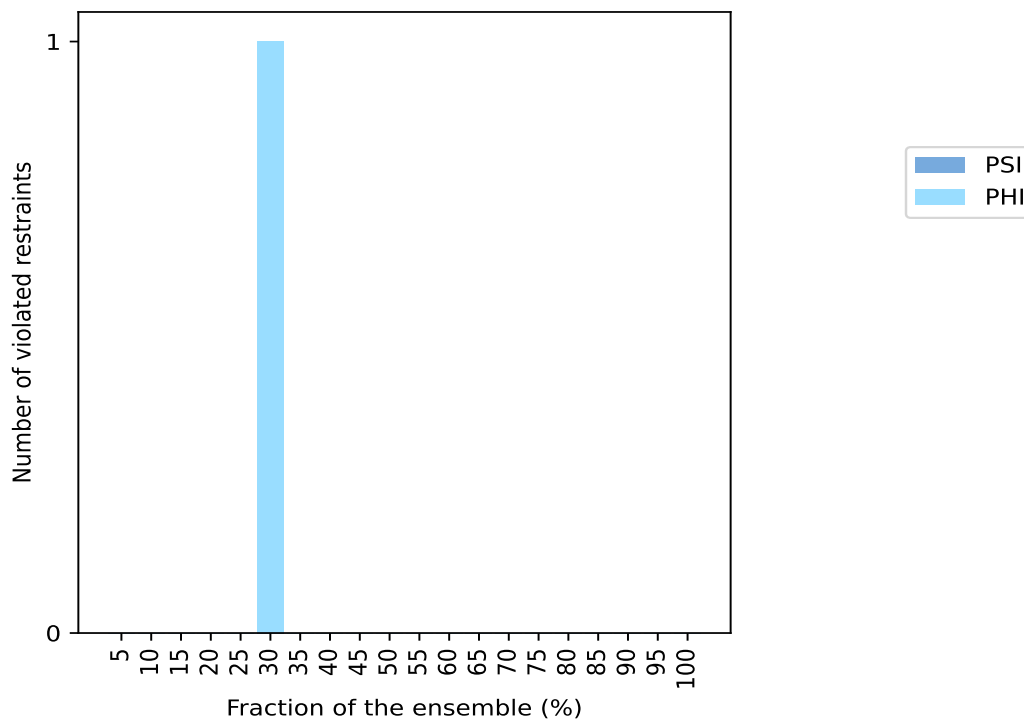
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 60.0 |
| 0 | 0 | 0 | 13 | 65.0 |
| 0 | 0 | 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](#)

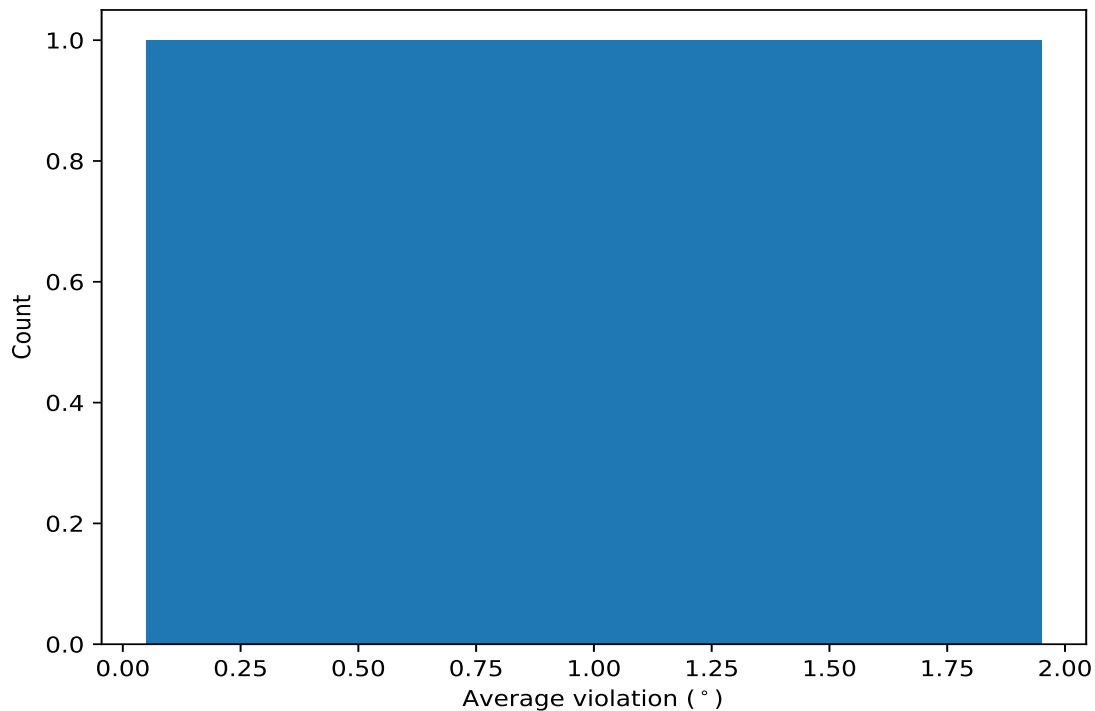


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

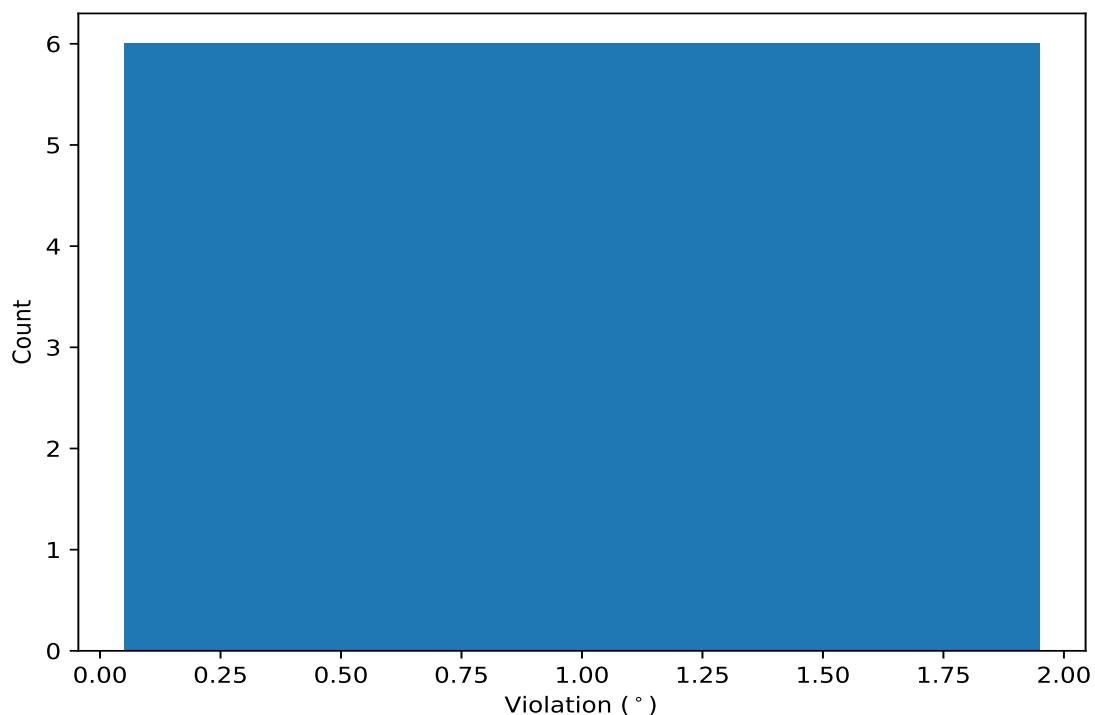
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|--------|--------------|--------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,99) | 1:A:64:PRO:C | 1:A:65:LEU:N | 1:A:65:LEU:CA | 1:A:65:LEU:C | 6 | 1.2 | 0.12 | 1.15 |

¹ Number of violated models, ²Standard 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 (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,99) | 1:A:64:PRO:C | 1:A:65:LEU:N | 1:A:65:LEU:CA | 1:A:65:LEU:C | 2 | 1.4 |
| (1,99) | 1:A:64:PRO:C | 1:A:65:LEU:N | 1:A:65:LEU:CA | 1:A:65:LEU:C | 16 | 1.3 |
| (1,99) | 1:A:64:PRO:C | 1:A:65:LEU:N | 1:A:65:LEU:CA | 1:A:65:LEU:C | 3 | 1.2 |
| (1,99) | 1:A:64:PRO:C | 1:A:65:LEU:N | 1:A:65:LEU:CA | 1:A:65:LEU:C | 9 | 1.1 |
| (1,99) | 1:A:64:PRO:C | 1:A:65:LEU:N | 1:A:65:LEU:CA | 1:A:65:LEU:C | 11 | 1.1 |
| (1,99) | 1:A:64:PRO:C | 1:A:65:LEU:N | 1:A:65:LEU:CA | 1:A:65:LEU:C | 20 | 1.1 |