



Full wwPDB NMR Structure Validation Report ⓘ

Jun 5, 2023 – 01:29 PM JST

PDB ID : 6LXG
BMRB ID : 36313
Title : NMR solution structure of regulatory ACT domain of the Mycobacterium tuberculosis Rel protein
Authors : Shin, J.; Singal, B.; Manimekalai, M.S.S.; Gruber, G.
Deposited on : 2020-02-11

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

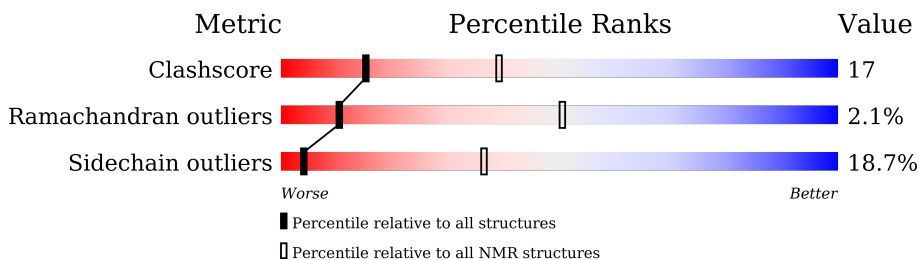
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 36%.

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 | 90 | 47% 37% • 12% |
| 1 | B | 90 | 43% 38% • 6% 12% |

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:1-A:75, B:2-B:75 (149) | 0.59 | 1 |

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. No single-model clusters were found.

| Cluster number | Models |
|----------------|-------------------------|
| 1 | 1, 6, 9, 16, 17, 19, 21 |
| 2 | 2, 4, 5, 7, 14 |
| 3 | 3, 8, 12, 13 |
| 4 | 11, 18, 20 |
| 5 | 10, 15 |

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2458 atoms, of which 1240 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GTP pyrophosphokinase.

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|-----|-----|-----|-----|-------|---|
| | | | Total | C | H | N | O | | S |
| 1 | A | 79 | 1229 | 379 | 620 | 112 | 117 | 1 | 0 |
| 1 | B | 79 | 1229 | 379 | 620 | 112 | 117 | 1 | 0 |

There are 22 discrepancies between the modelled and reference sequences:

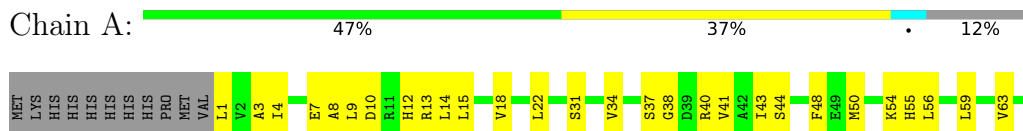
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|----------------|
| A | -10 | MET | - | initiating methionine | UNP A0A0U0QHY2 |
| A | -9 | LYS | - | expression tag | UNP A0A0U0QHY2 |
| A | -8 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| A | -7 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| A | -6 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| A | -5 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| A | -4 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| A | -3 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| A | -2 | PRO | - | expression tag | UNP A0A0U0QHY2 |
| A | -1 | MET | - | expression tag | UNP A0A0U0QHY2 |
| A | 0 | VAL | - | expression tag | UNP A0A0U0QHY2 |
| B | -10 | MET | - | initiating methionine | UNP A0A0U0QHY2 |
| B | -9 | LYS | - | expression tag | UNP A0A0U0QHY2 |
| B | -8 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| B | -7 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| B | -6 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| B | -5 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| B | -4 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| B | -3 | HIS | - | expression tag | UNP A0A0U0QHY2 |
| B | -2 | PRO | - | expression tag | UNP A0A0U0QHY2 |
| B | -1 | MET | - | expression tag | UNP A0A0U0QHY2 |
| B | 0 | VAL | - | expression tag | UNP A0A0U0QHY2 |

4 Residue-property plots [i](#)

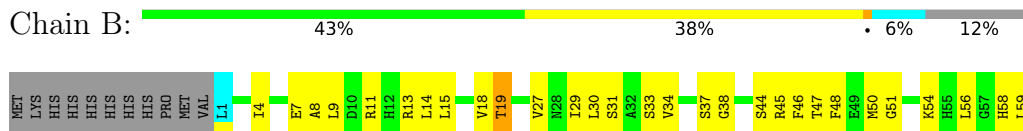
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: GTP pyrophosphokinase



- Molecule 1: GTP pyrophosphokinase

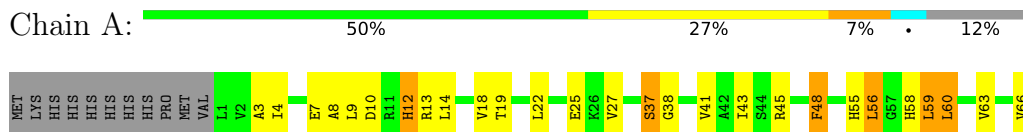


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: GTP pyrophosphokinase



T76
S77
A78
A79

- Molecule 1: GTP pyrophosphokinase

Chain B:  47% 30% 6% 6% 12%

MET LYS HIS HIS HIS HIS HIS HIS HIS PRO PRO MET MET VAL L1 V2 V3 A3 I4 E7 E8 H12 H13 L14 L15 S16 L17 D17 V18 T19 R20 K25 E26 V27 V28 H28 I29 L30 L31 V34 V37 G38 D39 R45 F46 T47 F48 E49 M50 G51 L56 L59 L60 L61 N61 A62 V63 E67 G68

V69 Y70 D71 V72 V75 T76 S77 A78 A79

4.2.2 Score per residue for model 2

- Molecule 1: GTP pyrophosphokinase

Chain A:  49% 31% 12%

MET LYS HIS HIS HIS HIS HIS HIS HIS PRO PRO MET MET VAL L1 E7 A8 L9 D10 R11 H12 H13 H14 L14 D17 V18 L22 V27 N28 V34 T36 S37 R40 V41 A42 I43 S44 R45 M50 G51 K54 H55 L56 L59 V63 V66 V69 Y70 D71 V72 Y73

T76
S77
A78
A79

- Molecule 1: GTP pyrophosphokinase

Chain B:  54% 24% 6% 12%

MET LYS HIS HIS HIS HIS HIS HIS HIS PRO PRO MET MET VAL L1 I4 A8 R11 H12 H13 L14 L15 T19 E25 K26 V27 N28 L29 L30 V34 F46 T47 F48 D52 P53 K54 H55 L56 L59 V63 R64 M65 V69 Y70 D71 V75 T76 S77 A78 A79

4.2.3 Score per residue for model 3

- Molecule 1: GTP pyrophosphokinase

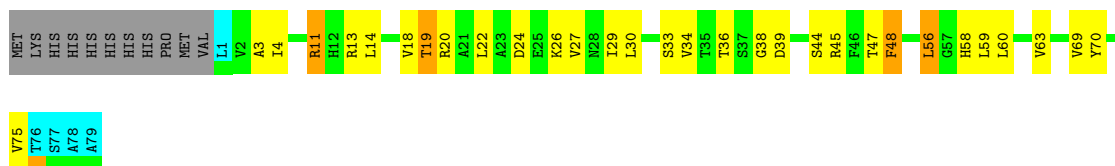
Chain A:  48% 34% 12%

MET LYS HIS HIS HIS HIS HIS HIS HIS PRO PRO MET MET VAL L1 V2 A3 I4 E7 A8 L9 D10 R11 H12 H13 R13 R13 R13 L14 L14 V18 L22 S31 V34 S37 G38 V41 A42 I43 S44 F48 E49 M50 G51 L56 G57 H58 L59 V63 R64 R65 V66 E67 G68 V69 Y70 D71

V72 T76 V75 S77 A78 A79

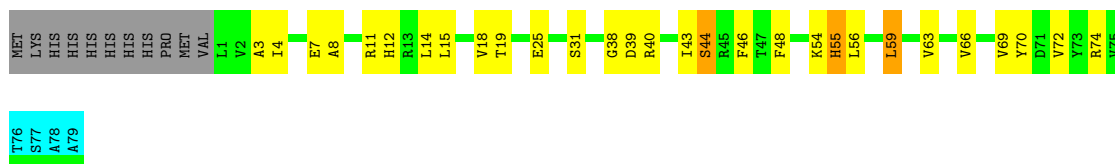
- Molecule 1: GTP pyrophosphokinase

Chain B:  48% 30% 6% 12%

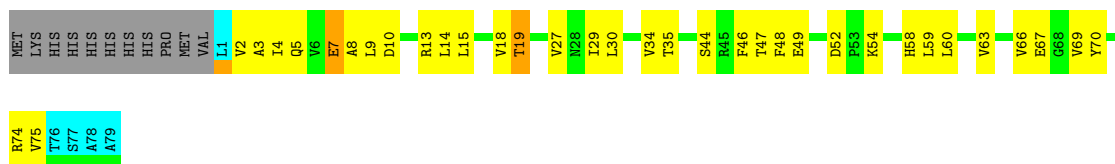


4.2.4 Score per residue for model 4

- Molecule 1: GTP pyrophosphokinase

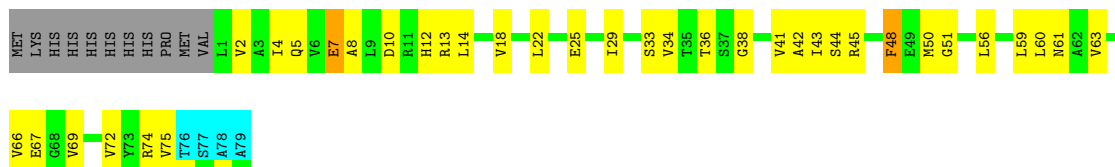


- Molecule 1: GTP pyrophosphokinase

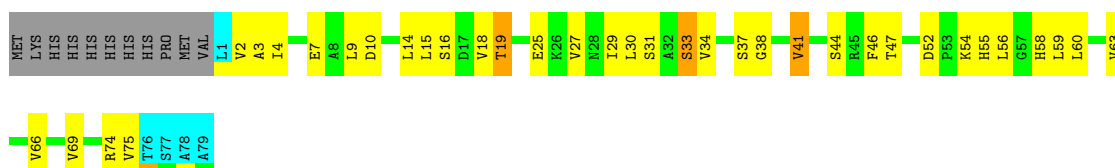


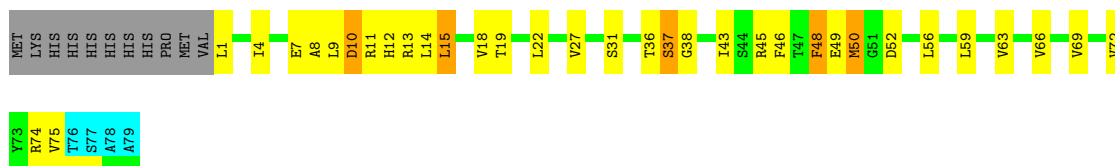
4.2.5 Score per residue for model 5

- Molecule 1: GTP pyrophosphokinase



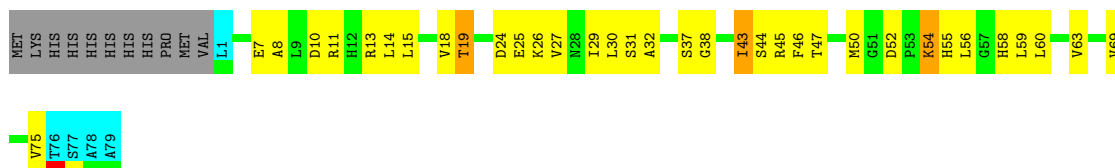
- Molecule 1: GTP pyrophosphokinase





- Molecule 1: GTP pyrophosphokinase

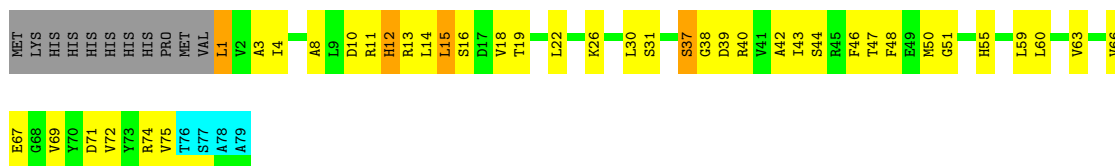
Chain B: 43% 36% 6% 12%



4.2.9 Score per residue for model 9

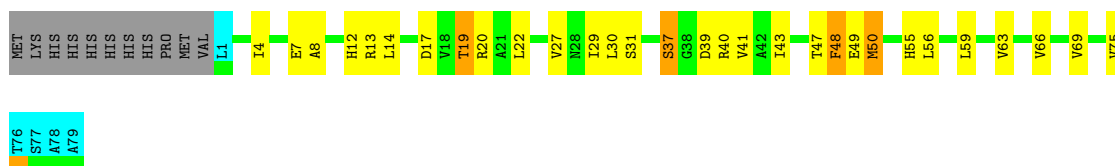
- Molecule 1: GTP pyrophosphokinase

Chain A: 39% 40% 12%



- Molecule 1: GTP pyrophosphokinase

Chain B: 49% 29% 6% 12%



4.2.10 Score per residue for model 10

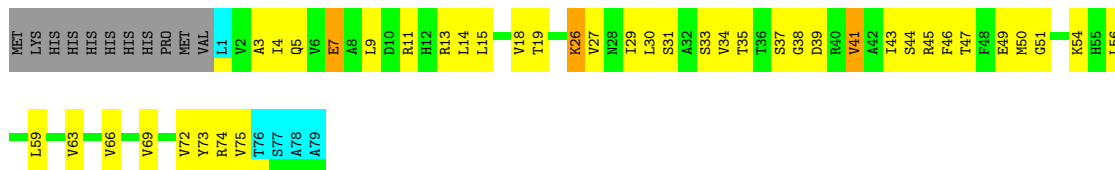
- Molecule 1: GTP pyrophosphokinase

Chain A: 48% 31% 12%



- Molecule 1: GTP pyrophosphokinase

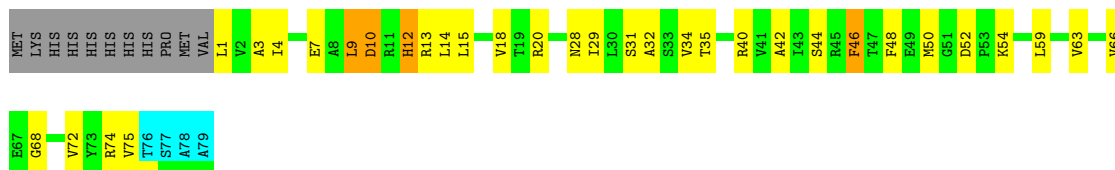
Chain B:



4.2.11 Score per residue for model 11

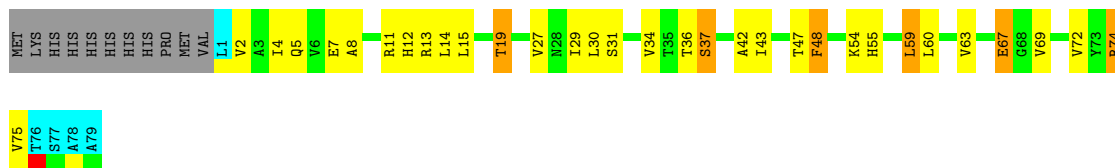
- Molecule 1: GTP pyrophosphokinase

Chain A:



- Molecule 1: GTP pyrophosphokinase

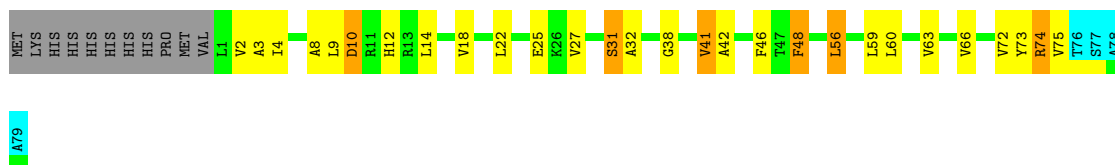
Chain B:



4.2.12 Score per residue for model 12

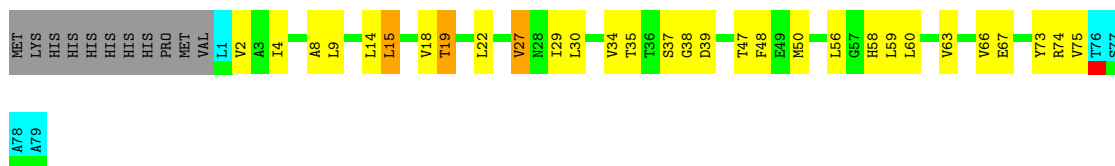
- Molecule 1: GTP pyrophosphokinase

Chain A:



- Molecule 1: GTP pyrophosphokinase

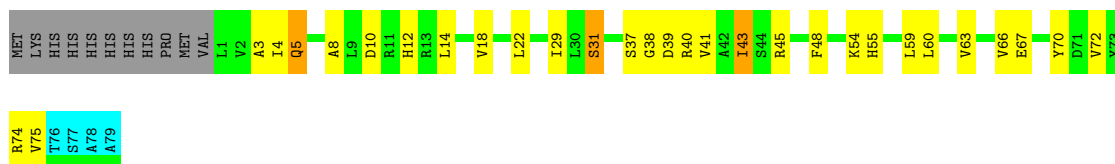
Chain B:



4.2.13 Score per residue for model 13

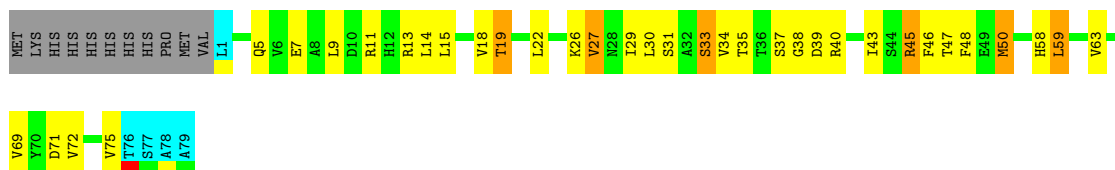
- Molecule 1: GTP pyrophosphokinase

Chain A: 50% 30% 12%



- Molecule 1: GTP pyrophosphokinase

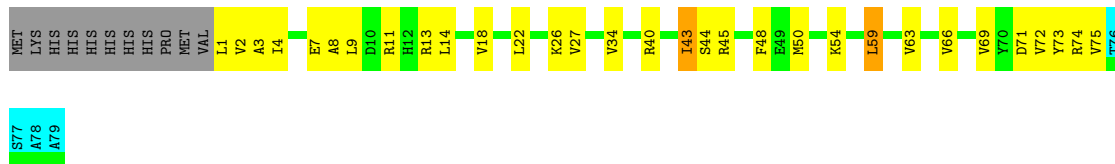
Chain B: 43% 32% 7% 6% 12%



4.2.14 Score per residue for model 14

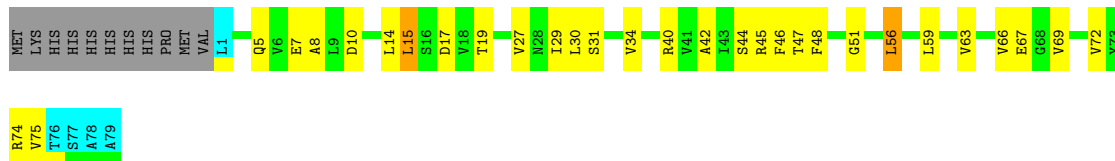
- Molecule 1: GTP pyrophosphokinase

Chain A: 49% 32% 12%



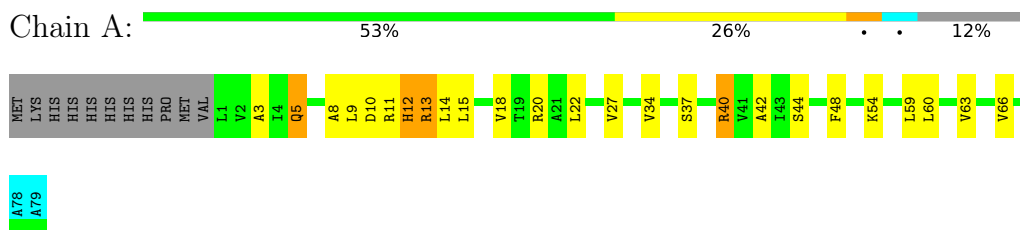
- Molecule 1: GTP pyrophosphokinase

Chain B: 49% 31% 6% 12%

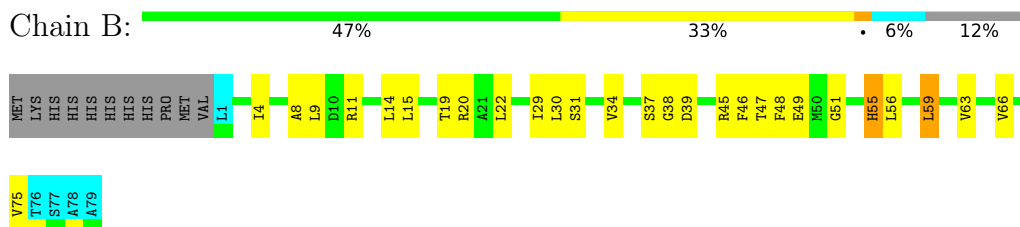


4.2.15 Score per residue for model 15

- Molecule 1: GTP pyrophosphokinase

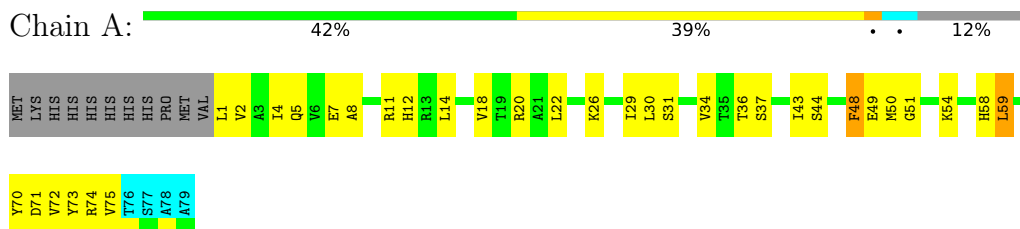


- Molecule 1: GTP pyrophosphokinase

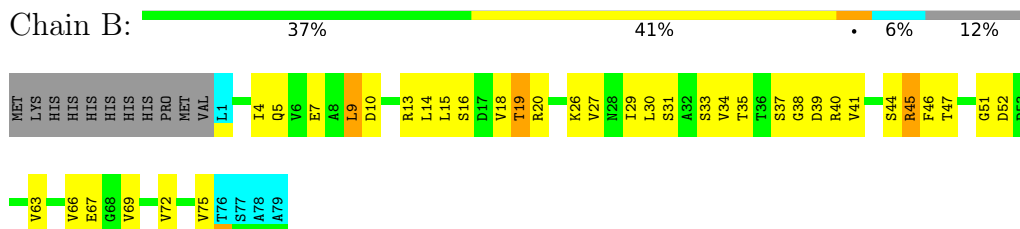


4.2.16 Score per residue for model 16

- Molecule 1: GTP pyrophosphokinase



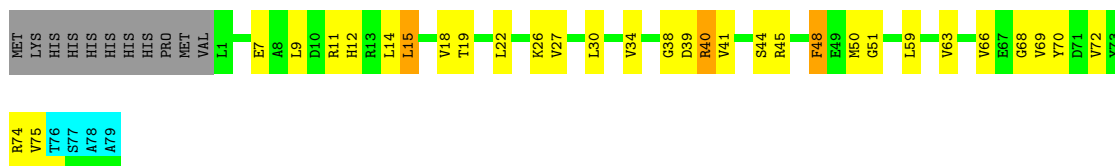
- Molecule 1: GTP pyrophosphokinase



4.2.17 Score per residue for model 17

- Molecule 1: GTP pyrophosphokinase





- Molecule 1: GTP pyrophosphokinase

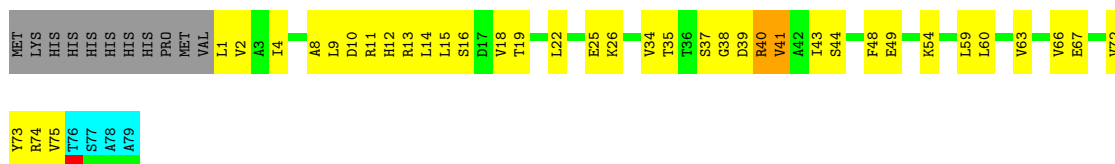
Chain B: 50% 29% 6% 12%



4.2.18 Score per residue for model 18

- Molecule 1: GTP pyrophosphokinase

Chain A: 41% 40% 12%



- Molecule 1: GTP pyrophosphokinase

Chain B: 38% 41% 6% 12%



4.2.19 Score per residue for model 19

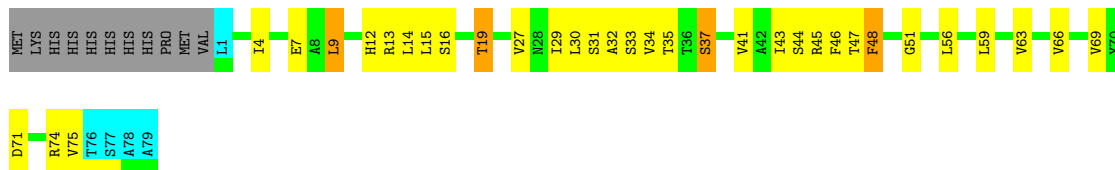
- Molecule 1: GTP pyrophosphokinase

Chain A: 38% 42% 12%



- Molecule 1: GTP pyrophosphokinase

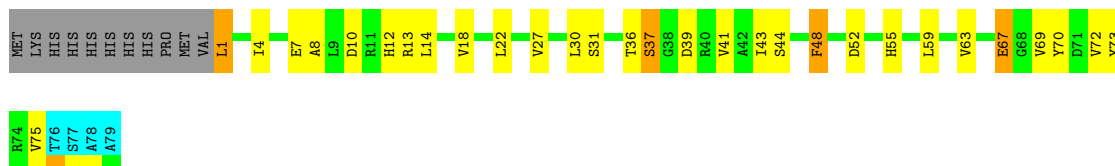
Chain B: 



4.2.20 Score per residue for model 20

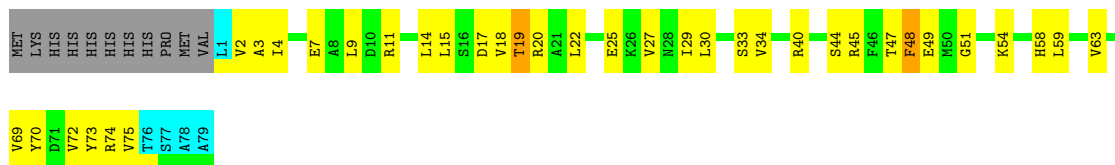
- Molecule 1: GTP pyrophosphokinase

Chain A: 



- Molecule 1: GTP pyrophosphokinase

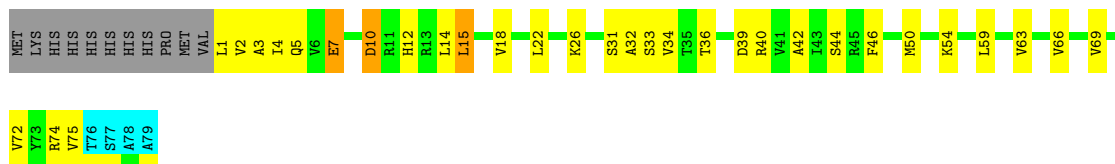
Chain B: 



4.2.21 Score per residue for model 21

- Molecule 1: GTP pyrophosphokinase

Chain A: 



- Molecule 1: GTP pyrophosphokinase

Chain B: 



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 21 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 |
|---------------|-----------------------|---------|
| CYANA | structure calculation | 2.1 |
| CNS | refinement | 1.2 |

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 | 776 |
| Number of shifts mapped to atoms | 776 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 36% |

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 | 585 | 598 | 597 | 22±3 |
| 1 | B | 577 | 587 | 584 | 21±3 |
| All | All | 24402 | 24885 | 24801 | 815 |

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

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:15:LEU:HD21 | 1:B:34:VAL:HG11 | 1.01 | 1.33 | 14 | 2 |
| 1:B:15:LEU:HD11 | 1:B:34:VAL:HG11 | 0.97 | 1.36 | 12 | 5 |
| 1:A:12:HIS:CD2 | 1:B:29:ILE:HD12 | 0.82 | 2.07 | 12 | 4 |
| 1:A:31:SER:CB | 1:B:35:THR:HG22 | 0.82 | 2.05 | 10 | 3 |
| 1:A:12:HIS:ND1 | 1:B:29:ILE:HD12 | 0.81 | 1.91 | 20 | 11 |
| 1:A:59:LEU:O | 1:A:63:VAL:HG23 | 0.80 | 1.77 | 10 | 21 |
| 1:B:59:LEU:O | 1:B:63:VAL:HG23 | 0.79 | 1.78 | 4 | 21 |
| 1:A:31:SER:OG | 1:B:35:THR:HG23 | 0.78 | 1.79 | 16 | 3 |
| 1:A:14:LEU:O | 1:A:18:VAL:HG23 | 0.77 | 1.78 | 3 | 21 |
| 1:A:9:LEU:HD13 | 1:A:40:ARG:O | 0.76 | 1.80 | 10 | 4 |
| 1:A:12:HIS:CD2 | 1:A:15:LEU:HD11 | 0.76 | 2.16 | 18 | 1 |
| 1:B:15:LEU:HD21 | 1:B:34:VAL:HG21 | 0.76 | 1.57 | 12 | 1 |
| 1:B:3:ALA:O | 1:B:4:ILE:HD13 | 0.74 | 1.82 | 7 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:4:ILE:HD11 | 1:B:48:PHE:CE1 | 0.73 | 2.17 | 19 | 6 |
| 1:B:15:LEU:HD11 | 1:B:34:VAL:CG1 | 0.73 | 2.13 | 12 | 5 |
| 1:A:3:ALA:O | 1:A:4:ILE:HD13 | 0.73 | 1.82 | 14 | 5 |
| 1:B:15:LEU:CD1 | 1:B:34:VAL:HG11 | 0.72 | 2.12 | 12 | 6 |
| 1:B:8:ALA:HB1 | 1:B:14:LEU:HD13 | 0.72 | 1.62 | 12 | 2 |
| 1:A:34:VAL:HG23 | 1:A:43:ILE:C | 0.71 | 2.05 | 14 | 8 |
| 1:B:38:GLY:N | 1:B:41:VAL:HG23 | 0.71 | 2.01 | 18 | 4 |
| 1:A:9:LEU:O | 1:A:14:LEU:HD12 | 0.70 | 1.86 | 14 | 9 |
| 1:B:39:ASP:O | 1:B:41:VAL:HG22 | 0.70 | 1.86 | 16 | 2 |
| 1:A:30:LEU:HB2 | 1:A:47:THR:HG23 | 0.70 | 1.61 | 9 | 1 |
| 1:B:8:ALA:HB1 | 1:B:14:LEU:HD22 | 0.70 | 1.64 | 21 | 1 |
| 1:B:37:SER:OG | 1:B:43:ILE:HD11 | 0.69 | 1.87 | 9 | 6 |
| 1:A:8:ALA:HB1 | 1:A:14:LEU:HD13 | 0.69 | 1.63 | 14 | 11 |
| 1:A:31:SER:HB3 | 1:B:35:THR:HG22 | 0.69 | 1.63 | 10 | 3 |
| 1:A:37:SER:OG | 1:A:43:ILE:HD11 | 0.69 | 1.88 | 7 | 9 |
| 1:A:56:LEU:O | 1:A:60:LEU:HD23 | 0.68 | 1.88 | 5 | 1 |
| 1:B:9:LEU:O | 1:B:14:LEU:HD12 | 0.68 | 1.89 | 19 | 8 |
| 1:B:3:ALA:C | 1:B:4:ILE:HD12 | 0.68 | 2.09 | 20 | 1 |
| 1:A:22:LEU:HD23 | 1:A:59:LEU:HD11 | 0.67 | 1.67 | 3 | 3 |
| 1:B:15:LEU:CD2 | 1:B:34:VAL:HG21 | 0.67 | 2.19 | 6 | 6 |
| 1:B:4:ILE:HD11 | 1:B:48:PHE:CE2 | 0.67 | 2.23 | 4 | 2 |
| 1:B:9:LEU:HD11 | 1:B:40:ARG:CG | 0.67 | 2.18 | 16 | 1 |
| 1:B:15:LEU:HD21 | 1:B:34:VAL:CG1 | 0.67 | 2.17 | 14 | 2 |
| 1:B:59:LEU:HD12 | 1:B:60:LEU:N | 0.67 | 2.04 | 4 | 1 |
| 1:B:55:HIS:O | 1:B:59:LEU:HD13 | 0.67 | 1.89 | 5 | 1 |
| 1:A:22:LEU:O | 1:A:27:VAL:HG22 | 0.67 | 1.89 | 14 | 1 |
| 1:A:55:HIS:O | 1:A:59:LEU:HD13 | 0.67 | 1.89 | 20 | 1 |
| 1:A:50:MET:CB | 1:A:56:LEU:HD21 | 0.66 | 2.20 | 8 | 1 |
| 1:B:30:LEU:HD11 | 1:B:49:GLU:HG2 | 0.66 | 1.66 | 21 | 1 |
| 1:A:31:SER:OG | 1:B:35:THR:HG22 | 0.65 | 1.90 | 12 | 2 |
| 1:A:34:VAL:HG12 | 1:A:44:SER:CB | 0.65 | 2.22 | 15 | 5 |
| 1:A:9:LEU:CD1 | 1:A:14:LEU:HD21 | 0.65 | 2.22 | 19 | 1 |
| 1:B:14:LEU:O | 1:B:18:VAL:HG23 | 0.65 | 1.91 | 12 | 13 |
| 1:A:10:ASP:OD1 | 1:A:36:THR:HG22 | 0.64 | 1.92 | 20 | 1 |
| 1:B:14:LEU:HD21 | 1:B:67:GLU:O | 0.64 | 1.91 | 11 | 7 |
| 1:A:12:HIS:CE1 | 1:B:19:THR:HG22 | 0.64 | 2.28 | 16 | 9 |
| 1:B:7:GLU:CG | 1:B:43:ILE:HD12 | 0.64 | 2.23 | 13 | 1 |
| 1:A:38:GLY:N | 1:A:41:VAL:HG23 | 0.64 | 2.07 | 13 | 5 |
| 1:B:14:LEU:HD21 | 1:B:68:GLY:HA3 | 0.64 | 1.69 | 21 | 1 |
| 1:B:48:PHE:CZ | 1:B:56:LEU:HD11 | 0.64 | 2.28 | 18 | 1 |
| 1:A:4:ILE:HD11 | 1:A:48:PHE:CE2 | 0.64 | 2.28 | 10 | 10 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:34:VAL:HG12 | 1:A:44:SER:HA | 0.64 | 1.68 | 17 | 5 |
| 1:B:8:ALA:HB1 | 1:B:14:LEU:HD23 | 0.63 | 1.70 | 9 | 1 |
| 1:B:5:GLN:HG3 | 1:B:75:VAL:HG21 | 0.63 | 1.70 | 21 | 2 |
| 1:B:4:ILE:HD11 | 1:B:56:LEU:CD2 | 0.63 | 2.24 | 3 | 1 |
| 1:A:15:LEU:CD1 | 1:A:34:VAL:HG11 | 0.63 | 2.22 | 17 | 1 |
| 1:B:15:LEU:CD2 | 1:B:34:VAL:HG11 | 0.62 | 2.19 | 14 | 3 |
| 1:B:3:ALA:HB3 | 1:B:75:VAL:O | 0.62 | 1.93 | 3 | 4 |
| 1:B:7:GLU:CA | 1:B:43:ILE:HD12 | 0.62 | 2.23 | 21 | 1 |
| 1:B:22:LEU:CD2 | 1:B:59:LEU:HD11 | 0.61 | 2.26 | 9 | 2 |
| 1:A:22:LEU:HD13 | 1:A:29:ILE:HD11 | 0.61 | 1.73 | 5 | 1 |
| 1:B:22:LEU:HD23 | 1:B:59:LEU:HD11 | 0.61 | 1.73 | 9 | 3 |
| 1:A:4:ILE:HD11 | 1:A:48:PHE:CE1 | 0.61 | 2.30 | 16 | 1 |
| 1:A:63:VAL:O | 1:A:66:VAL:HG23 | 0.61 | 1.94 | 17 | 19 |
| 1:A:31:SER:HB2 | 1:B:35:THR:HG22 | 0.60 | 1.73 | 10 | 1 |
| 1:A:32:ALA:HB2 | 1:A:46:PHE:CD1 | 0.60 | 2.31 | 21 | 3 |
| 1:A:22:LEU:HD23 | 1:A:59:LEU:HD22 | 0.60 | 1.73 | 15 | 1 |
| 1:B:8:ALA:HB1 | 1:B:14:LEU:HD21 | 0.60 | 1.71 | 15 | 3 |
| 1:B:5:GLN:O | 1:B:72:VAL:HG13 | 0.60 | 1.96 | 17 | 2 |
| 1:A:15:LEU:HD12 | 1:A:16:SER:N | 0.60 | 2.11 | 18 | 1 |
| 1:A:12:HIS:CG | 1:B:29:ILE:HD12 | 0.60 | 2.31 | 13 | 14 |
| 1:A:1:LEU:HD12 | 1:A:1:LEU:O | 0.60 | 1.97 | 6 | 3 |
| 1:B:50:MET:SD | 1:B:56:LEU:HD22 | 0.60 | 2.37 | 7 | 1 |
| 1:A:50:MET:HB3 | 1:A:56:LEU:HD21 | 0.59 | 1.74 | 8 | 1 |
| 1:B:52:ASP:O | 1:B:56:LEU:HD12 | 0.59 | 1.97 | 2 | 2 |
| 1:A:12:HIS:ND1 | 1:A:15:LEU:HD11 | 0.59 | 2.12 | 21 | 1 |
| 1:A:15:LEU:HD22 | 1:B:32:ALA:HB3 | 0.59 | 1.73 | 21 | 1 |
| 1:A:10:ASP:OD2 | 1:A:36:THR:HG22 | 0.59 | 1.98 | 5 | 2 |
| 1:A:56:LEU:HD23 | 1:A:56:LEU:O | 0.59 | 1.98 | 7 | 1 |
| 1:A:34:VAL:HG12 | 1:A:44:SER:HB3 | 0.59 | 1.75 | 11 | 3 |
| 1:A:48:PHE:CZ | 1:A:56:LEU:HD21 | 0.59 | 2.33 | 12 | 1 |
| 1:A:12:HIS:HB2 | 1:B:29:ILE:HD12 | 0.58 | 1.74 | 9 | 3 |
| 1:B:29:ILE:HD13 | 1:B:46:PHE:CD2 | 0.58 | 2.33 | 14 | 6 |
| 1:A:19:THR:HA | 1:A:22:LEU:HD12 | 0.58 | 1.75 | 9 | 4 |
| 1:B:4:ILE:HD12 | 1:B:48:PHE:CZ | 0.58 | 2.33 | 3 | 2 |
| 1:B:15:LEU:HD23 | 1:B:34:VAL:HG21 | 0.58 | 1.75 | 16 | 2 |
| 1:A:34:VAL:HG23 | 1:A:43:ILE:O | 0.58 | 1.99 | 19 | 4 |
| 1:B:56:LEU:HD23 | 1:B:56:LEU:O | 0.58 | 1.99 | 8 | 3 |
| 1:B:38:GLY:H | 1:B:41:VAL:HG23 | 0.57 | 1.59 | 16 | 3 |
| 1:A:5:GLN:O | 1:A:72:VAL:HG13 | 0.57 | 1.99 | 15 | 1 |
| 1:A:31:SER:HB3 | 1:B:35:THR:HG23 | 0.57 | 1.76 | 13 | 1 |
| 1:A:1:LEU:HD23 | 1:A:1:LEU:O | 0.57 | 2.00 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:11:ARG:HB2 | 1:B:14:LEU:HD12 | 0.57 | 1.77 | 21 | 2 |
| 1:B:15:LEU:HD22 | 1:B:34:VAL:HG11 | 0.56 | 1.77 | 13 | 5 |
| 1:B:8:ALA:O | 1:B:42:ALA:HB3 | 0.56 | 1.99 | 7 | 3 |
| 1:B:63:VAL:O | 1:B:66:VAL:HG23 | 0.56 | 1.99 | 15 | 11 |
| 1:B:37:SER:CB | 1:B:43:ILE:HD11 | 0.56 | 2.30 | 17 | 3 |
| 1:B:4:ILE:HD11 | 1:B:56:LEU:HD21 | 0.56 | 1.76 | 3 | 1 |
| 1:A:8:ALA:HB1 | 1:A:14:LEU:HG | 0.56 | 1.76 | 20 | 4 |
| 1:B:17:ASP:OD2 | 1:B:66:VAL:HG13 | 0.56 | 2.00 | 9 | 1 |
| 1:B:15:LEU:HD22 | 1:B:34:VAL:HG21 | 0.55 | 1.76 | 11 | 1 |
| 1:A:56:LEU:O | 1:A:60:LEU:HD12 | 0.55 | 2.00 | 1 | 1 |
| 1:A:12:HIS:NE2 | 1:B:19:THR:HG22 | 0.55 | 2.16 | 11 | 4 |
| 1:B:7:GLU:O | 1:B:69:VAL:HG13 | 0.55 | 1.99 | 11 | 14 |
| 1:A:2:VAL:HG13 | 1:A:74:ARG:NE | 0.55 | 2.17 | 18 | 2 |
| 1:A:63:VAL:HB | 1:A:72:VAL:HG21 | 0.55 | 1.78 | 4 | 1 |
| 1:B:9:LEU:O | 1:B:14:LEU:HD23 | 0.55 | 2.02 | 18 | 2 |
| 1:B:9:LEU:HD13 | 1:B:10:ASP:N | 0.55 | 2.16 | 16 | 1 |
| 1:A:22:LEU:HD13 | 1:A:29:ILE:CD1 | 0.55 | 2.32 | 5 | 1 |
| 1:A:29:ILE:HG21 | 1:A:46:PHE:CE1 | 0.55 | 2.36 | 11 | 1 |
| 1:A:22:LEU:CD2 | 1:A:59:LEU:HD11 | 0.55 | 2.32 | 18 | 2 |
| 1:A:15:LEU:HD12 | 1:B:19:THR:CG2 | 0.55 | 2.31 | 21 | 1 |
| 1:A:22:LEU:CD2 | 1:A:59:LEU:HD21 | 0.54 | 2.32 | 1 | 3 |
| 1:B:15:LEU:HD13 | 1:B:34:VAL:HG21 | 0.54 | 1.79 | 18 | 1 |
| 1:B:2:VAL:HG11 | 1:B:74:ARG:HD3 | 0.54 | 1.79 | 12 | 2 |
| 1:A:63:VAL:HG12 | 1:A:69:VAL:HG11 | 0.54 | 1.78 | 10 | 1 |
| 1:B:4:ILE:HD13 | 1:B:48:PHE:CE1 | 0.54 | 2.38 | 20 | 1 |
| 1:A:34:VAL:HG12 | 1:A:44:SER:CA | 0.54 | 2.33 | 21 | 5 |
| 1:B:22:LEU:HD22 | 1:B:59:LEU:HD21 | 0.54 | 1.80 | 9 | 1 |
| 1:A:14:LEU:HD11 | 1:A:67:GLU:O | 0.54 | 2.03 | 20 | 3 |
| 1:B:9:LEU:HD11 | 1:B:40:ARG:HG2 | 0.54 | 1.78 | 16 | 1 |
| 1:A:10:ASP:OD2 | 1:A:36:THR:HG23 | 0.53 | 2.03 | 8 | 1 |
| 1:B:63:VAL:CG1 | 1:B:72:VAL:HG21 | 0.53 | 2.34 | 14 | 5 |
| 1:A:19:THR:HG22 | 1:B:16:SER:OG | 0.53 | 2.02 | 19 | 1 |
| 1:B:4:ILE:HD11 | 1:B:48:PHE:HE1 | 0.53 | 1.60 | 19 | 3 |
| 1:A:10:ASP:OD2 | 1:A:42:ALA:HB2 | 0.53 | 2.04 | 5 | 2 |
| 1:A:63:VAL:CG1 | 1:A:72:VAL:HG21 | 0.53 | 2.34 | 11 | 7 |
| 1:A:12:HIS:HA | 1:A:15:LEU:HD21 | 0.53 | 1.81 | 9 | 2 |
| 1:B:7:GLU:HA | 1:B:43:ILE:HD12 | 0.53 | 1.81 | 21 | 1 |
| 1:A:8:ALA:HB2 | 1:A:69:VAL:HG22 | 0.52 | 1.81 | 5 | 12 |
| 1:A:9:LEU:HD23 | 1:A:68:GLY:CA | 0.52 | 2.34 | 11 | 1 |
| 1:A:34:VAL:HG23 | 1:A:44:SER:N | 0.52 | 2.18 | 14 | 3 |
| 1:A:7:GLU:O | 1:A:69:VAL:HG13 | 0.52 | 2.04 | 4 | 14 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:55:HIS:O | 1:B:59:LEU:HD23 | 0.52 | 2.03 | 15 | 1 |
| 1:B:63:VAL:HG11 | 1:B:72:VAL:HG21 | 0.52 | 1.80 | 18 | 6 |
| 1:B:41:VAL:O | 1:B:41:VAL:HG13 | 0.52 | 2.05 | 7 | 2 |
| 1:B:59:LEU:HD12 | 1:B:59:LEU:C | 0.52 | 2.25 | 4 | 1 |
| 1:A:5:GLN:HG3 | 1:A:75:VAL:HG21 | 0.52 | 1.80 | 5 | 1 |
| 1:B:7:GLU:HB3 | 1:B:43:ILE:HD12 | 0.52 | 1.82 | 8 | 1 |
| 1:A:22:LEU:HD13 | 1:A:29:ILE:HG12 | 0.52 | 1.81 | 13 | 3 |
| 1:B:3:ALA:HB3 | 1:B:75:VAL:C | 0.52 | 2.26 | 4 | 1 |
| 1:A:3:ALA:HB3 | 1:A:75:VAL:HB | 0.51 | 1.81 | 11 | 8 |
| 1:A:2:VAL:HG11 | 1:A:74:ARG:HD2 | 0.51 | 1.81 | 14 | 2 |
| 1:B:29:ILE:HG21 | 1:B:46:PHE:HB3 | 0.51 | 1.83 | 6 | 11 |
| 1:A:38:GLY:H | 1:A:41:VAL:HG23 | 0.51 | 1.65 | 13 | 7 |
| 1:A:15:LEU:HD11 | 1:A:44:SER:OG | 0.51 | 2.05 | 4 | 2 |
| 1:B:15:LEU:CG | 1:B:34:VAL:HG11 | 0.51 | 2.36 | 2 | 2 |
| 1:B:63:VAL:HG12 | 1:B:69:VAL:HG11 | 0.51 | 1.81 | 8 | 4 |
| 1:A:32:ALA:HB2 | 1:A:46:PHE:CE1 | 0.51 | 2.40 | 11 | 1 |
| 1:B:66:VAL:O | 1:B:69:VAL:HG12 | 0.51 | 2.06 | 15 | 1 |
| 1:A:22:LEU:HD23 | 1:A:59:LEU:HD21 | 0.51 | 1.83 | 1 | 2 |
| 1:A:2:VAL:HG11 | 1:A:74:ARG:CD | 0.50 | 2.35 | 14 | 2 |
| 1:A:7:GLU:CG | 1:A:43:ILE:HG23 | 0.50 | 2.35 | 14 | 1 |
| 1:A:63:VAL:HG11 | 1:A:72:VAL:CG2 | 0.50 | 2.37 | 7 | 2 |
| 1:A:12:HIS:HD2 | 1:A:15:LEU:HD11 | 0.50 | 1.61 | 18 | 1 |
| 1:A:19:THR:HG21 | 1:B:15:LEU:HD22 | 0.50 | 1.81 | 8 | 2 |
| 1:A:10:ASP:HA | 1:A:42:ALA:HB2 | 0.50 | 1.84 | 21 | 5 |
| 1:B:2:VAL:HG11 | 1:B:74:ARG:HD2 | 0.50 | 1.82 | 5 | 1 |
| 1:B:8:ALA:HB1 | 1:B:14:LEU:CD2 | 0.50 | 2.35 | 21 | 3 |
| 1:B:22:LEU:HD22 | 1:B:59:LEU:CD1 | 0.50 | 2.37 | 15 | 1 |
| 1:A:34:VAL:HG12 | 1:A:44:SER:OG | 0.50 | 2.07 | 21 | 1 |
| 1:B:48:PHE:CE2 | 1:B:56:LEU:HD11 | 0.50 | 2.41 | 18 | 1 |
| 1:A:63:VAL:HG11 | 1:A:72:VAL:HG21 | 0.50 | 1.82 | 2 | 11 |
| 1:A:22:LEU:CD1 | 1:A:29:ILE:HD11 | 0.50 | 2.37 | 5 | 1 |
| 1:B:30:LEU:N | 1:B:47:THR:O | 0.50 | 2.45 | 3 | 21 |
| 1:A:56:LEU:HD12 | 1:A:57:GLY:N | 0.49 | 2.22 | 3 | 1 |
| 1:B:34:VAL:HG13 | 1:B:34:VAL:O | 0.49 | 2.07 | 3 | 2 |
| 1:B:4:ILE:HD11 | 1:B:48:PHE:HE2 | 0.49 | 1.62 | 4 | 2 |
| 1:A:12:HIS:CD2 | 1:B:29:ILE:CD1 | 0.49 | 2.95 | 18 | 2 |
| 1:B:63:VAL:HG11 | 1:B:72:VAL:CG2 | 0.49 | 2.37 | 11 | 4 |
| 1:A:36:THR:O | 1:A:36:THR:HG23 | 0.49 | 2.07 | 10 | 1 |
| 1:B:29:ILE:HD13 | 1:B:46:PHE:CD1 | 0.49 | 2.42 | 19 | 3 |
| 1:A:30:LEU:HD11 | 1:A:49:GLU:HG3 | 0.48 | 1.85 | 16 | 1 |
| 1:B:18:VAL:HG12 | 1:B:46:PHE:CZ | 0.48 | 2.43 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:22:LEU:O | 1:A:27:VAL:HG23 | 0.48 | 2.08 | 8 | 8 |
| 1:A:14:LEU:HD22 | 1:A:67:GLU:O | 0.48 | 2.08 | 18 | 1 |
| 1:A:30:LEU:HD12 | 1:A:48:PHE:CA | 0.48 | 2.38 | 17 | 1 |
| 1:A:55:HIS:O | 1:A:59:LEU:HD12 | 0.48 | 2.08 | 4 | 1 |
| 1:B:9:LEU:HD11 | 1:B:40:ARG:HG3 | 0.48 | 1.86 | 16 | 1 |
| 1:A:29:ILE:HG21 | 1:A:46:PHE:HE1 | 0.48 | 1.68 | 11 | 1 |
| 1:B:29:ILE:HG22 | 1:B:47:THR:O | 0.48 | 2.09 | 20 | 1 |
| 1:A:12:HIS:CG | 1:B:29:ILE:CD1 | 0.47 | 2.97 | 13 | 10 |
| 1:A:12:HIS:CE1 | 1:B:29:ILE:HD12 | 0.47 | 2.43 | 3 | 2 |
| 1:B:15:LEU:HG | 1:B:34:VAL:HG21 | 0.47 | 1.85 | 19 | 1 |
| 1:A:9:LEU:HB2 | 1:A:14:LEU:HD11 | 0.47 | 1.85 | 14 | 2 |
| 1:B:33:SER:O | 1:B:45:ARG:N | 0.47 | 2.48 | 20 | 9 |
| 1:A:5:GLN:NE2 | 1:A:43:ILE:HG21 | 0.47 | 2.24 | 13 | 1 |
| 1:B:15:LEU:HD13 | 1:B:34:VAL:HG11 | 0.47 | 1.85 | 15 | 1 |
| 1:B:3:ALA:HB3 | 1:B:75:VAL:HB | 0.47 | 1.85 | 18 | 2 |
| 1:B:8:ALA:HB2 | 1:B:69:VAL:HG22 | 0.47 | 1.87 | 14 | 1 |
| 1:A:39:ASP:O | 1:A:41:VAL:HG23 | 0.47 | 2.10 | 20 | 1 |
| 1:B:9:LEU:O | 1:B:14:LEU:HD13 | 0.46 | 2.10 | 13 | 1 |
| 1:A:9:LEU:HD12 | 1:A:9:LEU:N | 0.46 | 2.25 | 19 | 1 |
| 1:A:1:LEU:HD21 | 1:A:47:THR:CG2 | 0.46 | 2.40 | 10 | 1 |
| 1:A:43:ILE:O | 1:A:43:ILE:HG23 | 0.46 | 2.10 | 6 | 3 |
| 1:A:12:HIS:CE1 | 1:B:27:VAL:N | 0.46 | 2.84 | 10 | 1 |
| 1:B:69:VAL:HG13 | 1:B:69:VAL:O | 0.46 | 2.11 | 15 | 1 |
| 1:A:9:LEU:HD12 | 1:A:40:ARG:O | 0.46 | 2.11 | 15 | 1 |
| 1:B:22:LEU:O | 1:B:27:VAL:HG23 | 0.46 | 2.10 | 12 | 2 |
| 1:B:4:ILE:HD12 | 1:B:46:PHE:O | 0.46 | 2.10 | 19 | 1 |
| 1:A:32:ALA:CB | 1:A:46:PHE:CE1 | 0.45 | 3.00 | 21 | 1 |
| 1:A:2:VAL:HG23 | 1:A:50:MET:CE | 0.45 | 2.42 | 16 | 1 |
| 1:A:1:LEU:HD21 | 1:A:47:THR:HG23 | 0.45 | 1.86 | 10 | 1 |
| 1:A:48:PHE:CD2 | 1:A:48:PHE:N | 0.45 | 2.83 | 20 | 1 |
| 1:B:48:PHE:CE1 | 1:B:50:MET:CG | 0.45 | 3.00 | 13 | 1 |
| 1:A:12:HIS:CE1 | 1:B:19:THR:CG2 | 0.45 | 2.99 | 6 | 4 |
| 1:B:4:ILE:HD11 | 1:B:48:PHE:CD1 | 0.45 | 2.45 | 19 | 1 |
| 1:B:12:HIS:O | 1:B:13:ARG:CB | 0.45 | 2.65 | 11 | 1 |
| 1:B:15:LEU:HD21 | 1:B:34:VAL:CB | 0.45 | 2.42 | 17 | 1 |
| 1:B:2:VAL:HG12 | 1:B:4:ILE:CD1 | 0.45 | 2.41 | 20 | 1 |
| 1:B:11:ARG:CB | 1:B:14:LEU:HD12 | 0.45 | 2.42 | 13 | 1 |
| 1:A:32:ALA:CB | 1:A:46:PHE:CD1 | 0.44 | 3.00 | 12 | 1 |
| 1:B:59:LEU:HD23 | 1:B:59:LEU:C | 0.44 | 2.32 | 19 | 1 |
| 1:B:48:PHE:CE1 | 1:B:56:LEU:HD11 | 0.44 | 2.47 | 14 | 1 |
| 1:A:48:PHE:CZ | 1:A:56:LEU:HD23 | 0.44 | 2.48 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:12:HIS:CD2 | 1:A:13:ARG:N | 0.44 | 2.85 | 15 | 1 |
| 1:B:22:LEU:CD2 | 1:B:59:LEU:HD21 | 0.44 | 2.41 | 9 | 1 |
| 1:A:32:ALA:HB1 | 1:A:45:ARG:O | 0.44 | 2.12 | 6 | 1 |
| 1:B:27:VAL:CG1 | 1:B:48:PHE:CD1 | 0.44 | 3.01 | 9 | 1 |
| 1:B:29:ILE:HG23 | 1:B:48:PHE:HB3 | 0.44 | 1.89 | 6 | 1 |
| 1:A:4:ILE:CD1 | 1:A:48:PHE:CE1 | 0.44 | 3.00 | 16 | 1 |
| 1:B:59:LEU:O | 1:B:59:LEU:HD13 | 0.44 | 2.13 | 18 | 1 |
| 1:A:1:LEU:HD13 | 1:A:47:THR:CG2 | 0.44 | 2.43 | 6 | 1 |
| 1:B:27:VAL:HG11 | 1:B:48:PHE:CE1 | 0.43 | 2.48 | 9 | 1 |
| 1:A:8:ALA:CB | 1:A:14:LEU:HD13 | 0.43 | 2.43 | 15 | 2 |
| 1:A:10:ASP:CG | 1:A:36:THR:HG22 | 0.43 | 2.33 | 5 | 1 |
| 1:A:1:LEU:HD23 | 1:A:30:LEU:HD13 | 0.43 | 1.89 | 9 | 1 |
| 1:B:50:MET:HE1 | 1:B:55:HIS:HB3 | 0.43 | 1.90 | 9 | 1 |
| 1:B:55:HIS:NE2 | 1:B:56:LEU:HD12 | 0.43 | 2.28 | 18 | 1 |
| 1:A:33:SER:HG | 1:B:33:SER:HB3 | 0.43 | 1.74 | 5 | 1 |
| 1:A:15:LEU:HD12 | 1:A:15:LEU:C | 0.43 | 2.34 | 18 | 1 |
| 1:A:4:ILE:CG2 | 1:A:72:VAL:CG1 | 0.43 | 2.96 | 20 | 9 |
| 1:A:12:HIS:ND1 | 1:B:29:ILE:CD1 | 0.43 | 2.80 | 21 | 2 |
| 1:A:4:ILE:CD1 | 1:A:48:PHE:CE2 | 0.43 | 3.02 | 7 | 2 |
| 1:B:48:PHE:CD1 | 1:B:48:PHE:N | 0.43 | 2.87 | 3 | 1 |
| 1:A:12:HIS:CE1 | 1:B:26:LYS:HA | 0.43 | 2.49 | 10 | 1 |
| 1:A:14:LEU:HD11 | 1:A:68:GLY:HA3 | 0.43 | 1.91 | 17 | 1 |
| 1:A:4:ILE:HD12 | 1:A:48:PHE:CE2 | 0.43 | 2.48 | 20 | 1 |
| 1:A:15:LEU:HD22 | 1:A:15:LEU:H | 0.42 | 1.74 | 17 | 1 |
| 1:B:37:SER:HB2 | 1:B:43:ILE:HD11 | 0.42 | 1.91 | 17 | 2 |
| 1:A:12:HIS:O | 1:A:12:HIS:CG | 0.42 | 2.73 | 21 | 1 |
| 1:B:8:ALA:HB2 | 1:B:69:VAL:HA | 0.42 | 1.91 | 2 | 1 |
| 1:B:48:PHE:CZ | 1:B:56:LEU:CD2 | 0.42 | 3.02 | 2 | 1 |
| 1:A:14:LEU:HD12 | 1:A:69:VAL:HG23 | 0.42 | 1.90 | 20 | 1 |
| 1:B:4:ILE:HD12 | 1:B:48:PHE:HZ | 0.42 | 1.71 | 3 | 2 |
| 1:A:39:ASP:O | 1:A:41:VAL:HG22 | 0.42 | 2.13 | 18 | 1 |
| 1:A:41:VAL:HG23 | 1:A:41:VAL:O | 0.42 | 2.14 | 5 | 1 |
| 1:A:7:GLU:HG2 | 1:A:43:ILE:HG23 | 0.42 | 1.92 | 14 | 1 |
| 1:B:55:HIS:O | 1:B:59:LEU:HD12 | 0.42 | 2.15 | 8 | 1 |
| 1:A:9:LEU:HD22 | 1:A:11:ARG:HH21 | 0.42 | 1.75 | 19 | 1 |
| 1:A:15:LEU:HG | 1:B:32:ALA:HB3 | 0.42 | 1.92 | 19 | 1 |
| 1:A:22:LEU:CD2 | 1:A:59:LEU:HD22 | 0.42 | 2.44 | 15 | 1 |
| 1:A:37:SER:HB2 | 1:A:43:ILE:HD11 | 0.42 | 1.92 | 13 | 1 |
| 1:B:50:MET:CG | 1:B:56:LEU:HD13 | 0.41 | 2.46 | 1 | 1 |
| 1:A:52:ASP:O | 1:A:55:HIS:CD2 | 0.41 | 2.73 | 10 | 1 |
| 1:B:15:LEU:HD11 | 1:B:34:VAL:CB | 0.41 | 2.45 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:55:HIS:ND1 | 1:B:56:LEU:N | 0.41 | 2.68 | 16 | 1 |
| 1:B:55:HIS:CD2 | 1:B:56:LEU:N | 0.41 | 2.88 | 18 | 1 |
| 1:B:4:ILE:HD11 | 1:B:48:PHE:CD2 | 0.41 | 2.50 | 4 | 1 |
| 1:A:50:MET:HB2 | 1:A:56:LEU:HD21 | 0.41 | 1.91 | 8 | 1 |
| 1:B:4:ILE:CG2 | 1:B:72:VAL:CG1 | 0.41 | 2.98 | 16 | 3 |
| 1:A:9:LEU:CD1 | 1:A:14:LEU:CD2 | 0.41 | 2.98 | 19 | 1 |
| 1:A:25:GLU:O | 1:A:26:LYS:CG | 0.41 | 2.69 | 19 | 1 |
| 1:B:7:GLU:CB | 1:B:43:ILE:HD12 | 0.41 | 2.45 | 8 | 1 |
| 1:A:12:HIS:CD2 | 1:B:27:VAL:O | 0.41 | 2.74 | 9 | 1 |
| 1:B:50:MET:HG3 | 1:B:56:LEU:HD12 | 0.41 | 1.93 | 10 | 1 |
| 1:A:22:LEU:HD21 | 1:A:59:LEU:HD21 | 0.41 | 1.91 | 21 | 1 |
| 1:B:22:LEU:HD13 | 1:B:29:ILE:HD11 | 0.41 | 1.92 | 3 | 1 |
| 1:B:3:ALA:O | 1:B:4:ILE:HD12 | 0.41 | 2.15 | 20 | 1 |
| 1:A:55:HIS:ND1 | 1:A:56:LEU:N | 0.41 | 2.69 | 6 | 3 |
| 1:A:46:PHE:CD2 | 1:A:46:PHE:O | 0.41 | 2.74 | 4 | 2 |
| 1:A:12:HIS:CE1 | 1:B:19:THR:HG23 | 0.41 | 2.50 | 20 | 2 |
| 1:A:50:MET:SD | 1:A:56:LEU:HD22 | 0.41 | 2.56 | 2 | 1 |
| 1:A:14:LEU:HD21 | 1:A:67:GLU:O | 0.41 | 2.16 | 7 | 1 |
| 1:A:48:PHE:CZ | 1:A:56:LEU:CD2 | 0.41 | 3.04 | 8 | 1 |
| 1:B:54:LYS:O | 1:B:58:HIS:CD2 | 0.41 | 2.74 | 8 | 1 |
| 1:B:39:ASP:O | 1:B:41:VAL:HG23 | 0.41 | 2.15 | 9 | 1 |
| 1:A:9:LEU:HD23 | 1:A:68:GLY:HA3 | 0.41 | 1.91 | 11 | 1 |
| 1:A:11:ARG:NH1 | 1:B:28:ASN:ND2 | 0.41 | 2.69 | 18 | 1 |
| 1:A:45:ARG:O | 1:A:46:PHE:CD2 | 0.41 | 2.74 | 8 | 1 |
| 1:A:12:HIS:HE1 | 1:B:19:THR:HG22 | 0.40 | 1.73 | 5 | 1 |
| 1:B:2:VAL:CG1 | 1:B:74:ARG:CD | 0.40 | 3.00 | 5 | 1 |
| 1:B:29:ILE:CD1 | 1:B:46:PHE:CD2 | 0.40 | 3.04 | 5 | 1 |
| 1:A:25:GLU:HB3 | 1:A:27:VAL:HG23 | 0.40 | 1.92 | 7 | 1 |
| 1:B:2:VAL:CG1 | 1:B:74:ARG:CG | 0.40 | 2.99 | 5 | 2 |
| 1:A:52:ASP:O | 1:A:55:HIS:CE1 | 0.40 | 2.74 | 7 | 1 |
| 1:A:5:GLN:NE2 | 1:A:43:ILE:CG2 | 0.40 | 2.84 | 13 | 1 |
| 1:A:2:VAL:CG1 | 1:A:74:ARG:CG | 0.40 | 2.99 | 21 | 1 |
| 1:A:2:VAL:HG23 | 1:A:50:MET:HE2 | 0.40 | 1.94 | 16 | 1 |
| 1:B:4:ILE:HG23 | 1:B:72:VAL:CG1 | 0.40 | 2.47 | 20 | 1 |
| 1:B:50:MET:CG | 1:B:56:LEU:CD1 | 0.40 | 2.99 | 6 | 1 |
| 1:A:15:LEU:HD13 | 1:B:32:ALA:HB3 | 0.40 | 1.92 | 8 | 1 |
| 1:A:8:ALA:HB2 | 1:A:69:VAL:HA | 0.40 | 1.93 | 10 | 1 |
| 1:B:2:VAL:HG11 | 1:B:74:ARG:CD | 0.40 | 2.44 | 12 | 1 |
| 1:A:50:MET:CE | 1:A:56:LEU:CD2 | 0.40 | 3.00 | 3 | 1 |
| 1:B:18:VAL:CG1 | 1:B:46:PHE:CZ | 0.40 | 3.04 | 8 | 1 |
| 1:A:16:SER:CB | 1:B:19:THR:CG2 | 0.40 | 3.00 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:22:LEU:HB3 | 1:A:27:VAL:HG23 | 0.40 | 1.93 | 14 | 1 |
| 1:B:63:VAL:HB | 1:B:72:VAL:HG21 | 0.40 | 1.93 | 15 | 1 |
| 1:A:1:LEU:HD11 | 1:A:30:LEU:HD13 | 0.40 | 1.92 | 20 | 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 | 74/90 (82%) | 69±1 (94±2%) | 4±2 (5±2%) | 1±1 (1±1%) | 15 | 61 |
| 1 | B | 74/90 (82%) | 67±1 (91±2%) | 5±1 (7±2%) | 2±1 (3±1%) | 8 | 42 |
| All | All | 3108/3780 (82%) | 2865 (92%) | 178 (6%) | 65 (2%) | 10 | 50 |

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 27 | VAL | 18 |
| 1 | B | 51 | GLY | 12 |
| 1 | A | 10 | ASP | 11 |
| 1 | A | 51 | GLY | 6 |
| 1 | B | 38 | GLY | 6 |
| 1 | A | 38 | GLY | 4 |
| 1 | B | 10 | ASP | 4 |
| 1 | B | 13 | ARG | 2 |
| 1 | A | 39 | ASP | 1 |
| 1 | B | 39 | ASP | 1 |

6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1 | A | 64/77 (83%) | 52±2 (82±4%) | 12±2 (18±4%) | 4 | 37 |
| 1 | B | 63/77 (82%) | 51±2 (81±3%) | 12±2 (19±3%) | 4 | 35 |
| All | All | 2667/3234 (82%) | 2168 (81%) | 499 (19%) | 4 | 36 |

All 90 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 | B | 19 | THR | 20 |
| 1 | B | 31 | SER | 16 |
| 1 | A | 48 | PHE | 14 |
| 1 | B | 37 | SER | 13 |
| 1 | A | 40 | ARG | 12 |
| 1 | A | 54 | LYS | 12 |
| 1 | B | 44 | SER | 12 |
| 1 | A | 13 | ARG | 11 |
| 1 | A | 37 | SER | 10 |
| 1 | B | 54 | LYS | 10 |
| 1 | B | 58 | HIS | 10 |
| 1 | A | 74 | ARG | 10 |
| 1 | A | 70 | TYR | 9 |
| 1 | B | 70 | TYR | 9 |
| 1 | A | 50 | MET | 9 |
| 1 | B | 11 | ARG | 9 |
| 1 | B | 13 | ARG | 9 |
| 1 | A | 45 | ARG | 8 |
| 1 | A | 60 | LEU | 8 |
| 1 | B | 20 | ARG | 8 |
| 1 | A | 1 | LEU | 8 |
| 1 | B | 56 | LEU | 8 |
| 1 | B | 45 | ARG | 7 |
| 1 | B | 48 | PHE | 7 |
| 1 | B | 60 | LEU | 7 |
| 1 | A | 44 | SER | 7 |
| 1 | A | 73 | TYR | 7 |
| 1 | A | 31 | SER | 7 |
| 1 | B | 26 | LYS | 7 |
| 1 | A | 11 | ARG | 7 |
| 1 | B | 74 | ARG | 7 |
| 1 | A | 26 | LYS | 7 |
| 1 | A | 25 | GLU | 6 |
| 1 | A | 59 | LEU | 6 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 25 | GLU | 6 |
| 1 | B | 50 | MET | 6 |
| 1 | B | 52 | ASP | 6 |
| 1 | B | 5 | GLN | 6 |
| 1 | B | 49 | GLU | 6 |
| 1 | B | 73 | TYR | 6 |
| 1 | A | 15 | LEU | 6 |
| 1 | A | 12 | HIS | 5 |
| 1 | A | 55 | HIS | 5 |
| 1 | B | 15 | LEU | 5 |
| 1 | B | 17 | ASP | 5 |
| 1 | B | 59 | LEU | 5 |
| 1 | A | 7 | GLU | 5 |
| 1 | A | 67 | GLU | 5 |
| 1 | A | 39 | ASP | 5 |
| 1 | A | 5 | GLN | 5 |
| 1 | B | 40 | ARG | 5 |
| 1 | A | 56 | LEU | 4 |
| 1 | B | 12 | HIS | 4 |
| 1 | B | 39 | ASP | 4 |
| 1 | A | 28 | ASN | 4 |
| 1 | A | 41 | VAL | 4 |
| 1 | A | 71 | ASP | 4 |
| 1 | A | 20 | ARG | 4 |
| 1 | A | 58 | HIS | 3 |
| 1 | A | 17 | ASP | 3 |
| 1 | A | 36 | THR | 3 |
| 1 | B | 71 | ASP | 3 |
| 1 | B | 36 | THR | 3 |
| 1 | B | 16 | SER | 3 |
| 1 | A | 49 | GLU | 3 |
| 1 | B | 55 | HIS | 3 |
| 1 | A | 52 | ASP | 3 |
| 1 | A | 35 | THR | 3 |
| 1 | B | 14 | LEU | 2 |
| 1 | A | 64 | ARG | 2 |
| 1 | B | 24 | ASP | 2 |
| 1 | B | 7 | GLU | 2 |
| 1 | B | 33 | SER | 2 |
| 1 | B | 41 | VAL | 2 |
| 1 | A | 33 | SER | 2 |
| 1 | A | 9 | LEU | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 43 | ILE | 2 |
| 1 | B | 9 | LEU | 2 |
| 1 | B | 61 | ASN | 1 |
| 1 | B | 65 | ASN | 1 |
| 1 | A | 61 | ASN | 1 |
| 1 | A | 24 | ASP | 1 |
| 1 | B | 43 | ILE | 1 |
| 1 | A | 65 | ASN | 1 |
| 1 | A | 46 | PHE | 1 |
| 1 | B | 67 | GLU | 1 |
| 1 | A | 10 | ASP | 1 |
| 1 | B | 10 | ASP | 1 |
| 1 | B | 28 | ASN | 1 |
| 1 | B | 64 | ARG | 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 36% for the well-defined parts and 36% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *deposit_mtrel_act.bmr*

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 | 776 |
| Number of shifts mapped to atoms | 776 |
| 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 |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 73 | -0.06 ± 0.16 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 65 | 0.12 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 61 | 0.00 ± 0.49 | 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 36%, i.e. 757 atoms were assigned a chemical shift out of a possible 2076. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone | 261/749 (35%) | 131/304 (43%) | 70/298 (23%) | 60/147 (41%) |
| Sidechain | 487/1203 (40%) | 344/787 (44%) | 140/362 (39%) | 3/54 (6%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 9/124 (7%) | 9/60 (15%) | 0/52 (0%) | 0/12 (0%) |
| Overall | 757/2076 (36%) | 484/1151 (42%) | 210/712 (29%) | 63/213 (30%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 776 atoms were assigned a chemical shift out of a possible 2168. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone | 269/794 (34%) | 135/322 (42%) | 73/316 (23%) | 61/156 (39%) |
| Sidechain | 498/1250 (40%) | 352/820 (43%) | 143/376 (38%) | 3/54 (6%) |
| Aromatic | 9/124 (7%) | 9/60 (15%) | 0/52 (0%) | 0/12 (0%) |
| Overall | 776/2168 (36%) | 496/1202 (41%) | 216/744 (29%) | 64/222 (29%) |

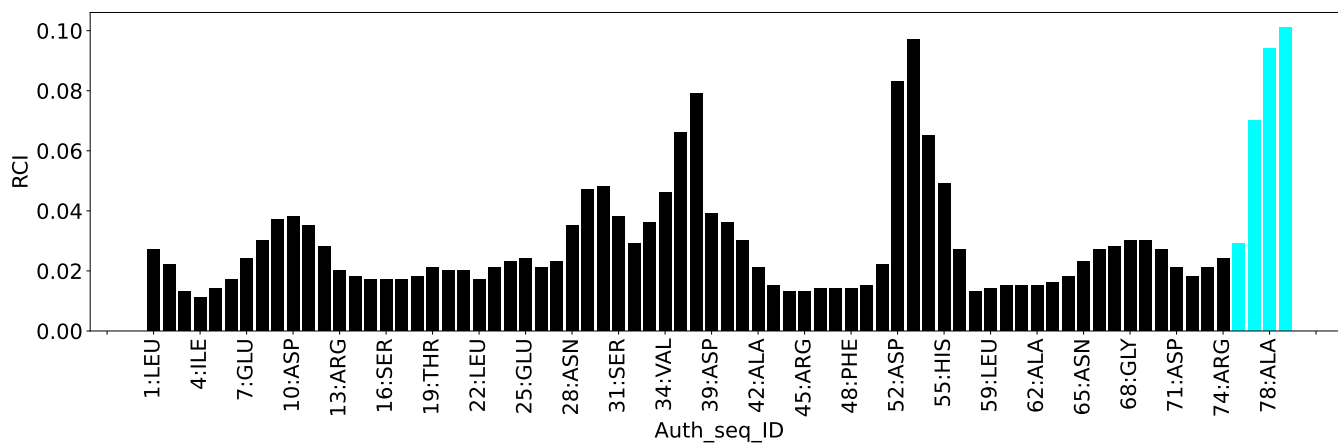
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

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 | 2510 |
| Intra-residue ($ i-j =0$) | 722 |
| Sequential ($ i-j =1$) | 562 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 336 |
| Long range ($ i-j \geq 5$) | 698 |
| Inter-chain | 60 |
| Hydrogen bond restraints | 132 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 246 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 15.3 |
| Number of long range restraints per residue ¹ | 4.3 |

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) | 26.9 | 0.12 |
| 0.2-0.5 (Medium) | 2.0 | 0.38 |
| >0.5 (Large) | 4.0 | 0.55 |

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) | 1.0 | 2.1 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis [i](#)

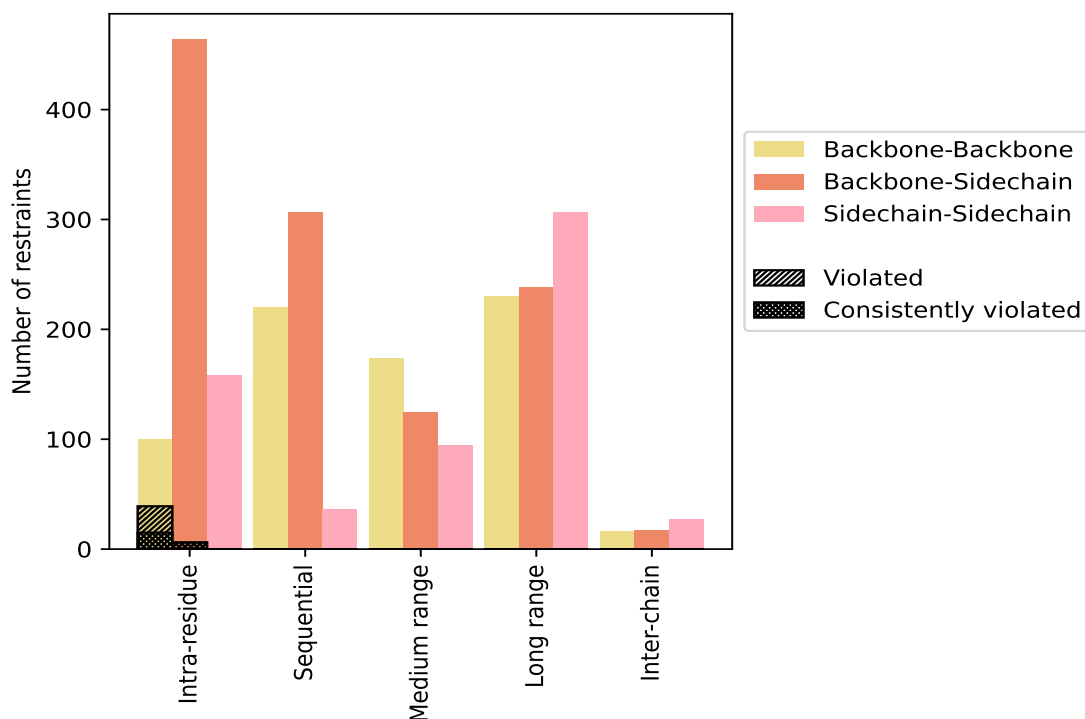
9.1 Summary of distance violations [i](#)

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 ($i-j =0$) | 722 | 28.8 | 45 | 6.2 | 1.8 | 21 | 2.9 | 0.8 |
| Backbone-Backbone | 100 | 4.0 | 39 | 39.0 | 1.6 | 15 | 15.0 | 0.6 |
| Backbone-Sidechain | 464 | 18.5 | 6 | 1.3 | 0.2 | 6 | 1.3 | 0.2 |
| Sidechain-Sidechain | 158 | 6.3 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sequential ($i-j =1$) | 562 | 22.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 220 | 8.8 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 306 | 12.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 36 | 1.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Medium range ($i-j >1$ & $i-j <5$) | 336 | 13.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 118 | 4.7 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 124 | 4.9 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 94 | 3.7 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Long range ($i-j \geq 5$) | 698 | 27.8 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 154 | 6.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 238 | 9.5 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 306 | 12.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Inter-chain | 60 | 2.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 16 | 0.6 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 17 | 0.7 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 27 | 1.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 132 | 5.3 | 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 | 2510 | 100.0 | 45 | 1.8 | 1.8 | 21 | 0.8 | 0.8 |
| Backbone-Backbone | 740 | 29.5 | 39 | 5.3 | 1.6 | 15 | 2.0 | 0.6 |
| Backbone-Sidechain | 1149 | 45.8 | 6 | 0.5 | 0.2 | 6 | 0.5 | 0.2 |
| Sidechain-Sidechain | 621 | 24.7 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |

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 | 30 | 0 | 0 | 0 | 0 | 30 | 0.19 | 0.54 | 0.15 | 0.12 |
| 2 | 37 | 0 | 0 | 0 | 0 | 37 | 0.17 | 0.54 | 0.14 | 0.12 |
| 3 | 36 | 0 | 0 | 0 | 0 | 36 | 0.18 | 0.54 | 0.14 | 0.12 |
| 4 | 33 | 0 | 0 | 0 | 0 | 33 | 0.18 | 0.54 | 0.14 | 0.11 |
| 5 | 35 | 0 | 0 | 0 | 0 | 35 | 0.18 | 0.54 | 0.14 | 0.12 |
| 6 | 27 | 0 | 0 | 0 | 0 | 27 | 0.2 | 0.54 | 0.16 | 0.12 |
| 7 | 34 | 0 | 0 | 0 | 0 | 34 | 0.18 | 0.55 | 0.14 | 0.12 |
| 8 | 36 | 0 | 0 | 0 | 0 | 36 | 0.17 | 0.54 | 0.14 | 0.11 |
| 9 | 31 | 0 | 0 | 0 | 0 | 31 | 0.18 | 0.53 | 0.14 | 0.12 |
| 10 | 33 | 0 | 0 | 0 | 0 | 33 | 0.18 | 0.54 | 0.14 | 0.12 |
| 11 | 34 | 0 | 0 | 0 | 0 | 34 | 0.18 | 0.54 | 0.14 | 0.12 |

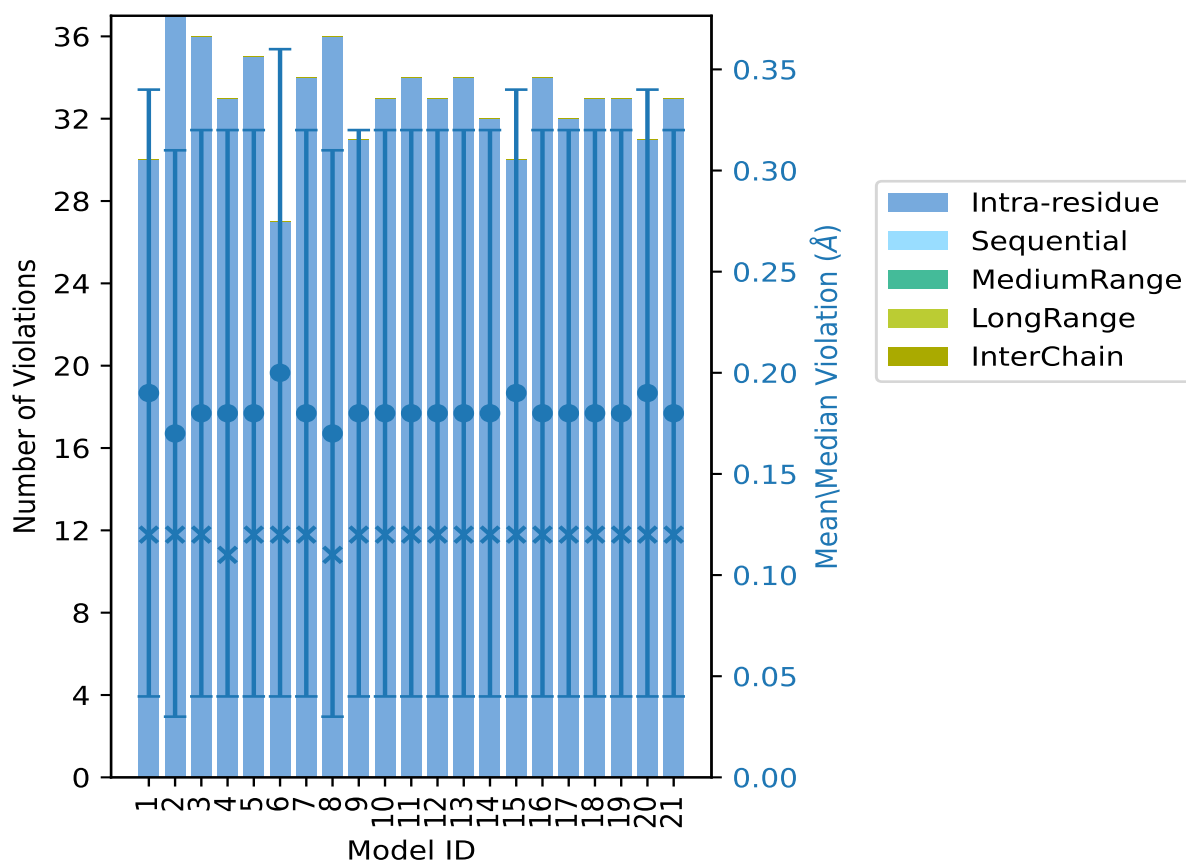
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 12 | 33 | 0 | 0 | 0 | 0 | 33 | 0.18 | 0.53 | 0.14 | 0.12 |
| 13 | 34 | 0 | 0 | 0 | 0 | 34 | 0.18 | 0.53 | 0.14 | 0.12 |
| 14 | 32 | 0 | 0 | 0 | 0 | 32 | 0.18 | 0.53 | 0.14 | 0.12 |
| 15 | 30 | 0 | 0 | 0 | 0 | 30 | 0.19 | 0.55 | 0.15 | 0.12 |
| 16 | 34 | 0 | 0 | 0 | 0 | 34 | 0.18 | 0.54 | 0.14 | 0.12 |
| 17 | 32 | 0 | 0 | 0 | 0 | 32 | 0.18 | 0.54 | 0.14 | 0.12 |
| 18 | 33 | 0 | 0 | 0 | 0 | 33 | 0.18 | 0.54 | 0.14 | 0.12 |
| 19 | 33 | 0 | 0 | 0 | 0 | 33 | 0.18 | 0.54 | 0.14 | 0.12 |
| 20 | 31 | 0 | 0 | 0 | 0 | 31 | 0.19 | 0.54 | 0.15 | 0.12 |
| 21 | 33 | 0 | 0 | 0 | 0 | 33 | 0.18 | 0.53 | 0.14 | 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

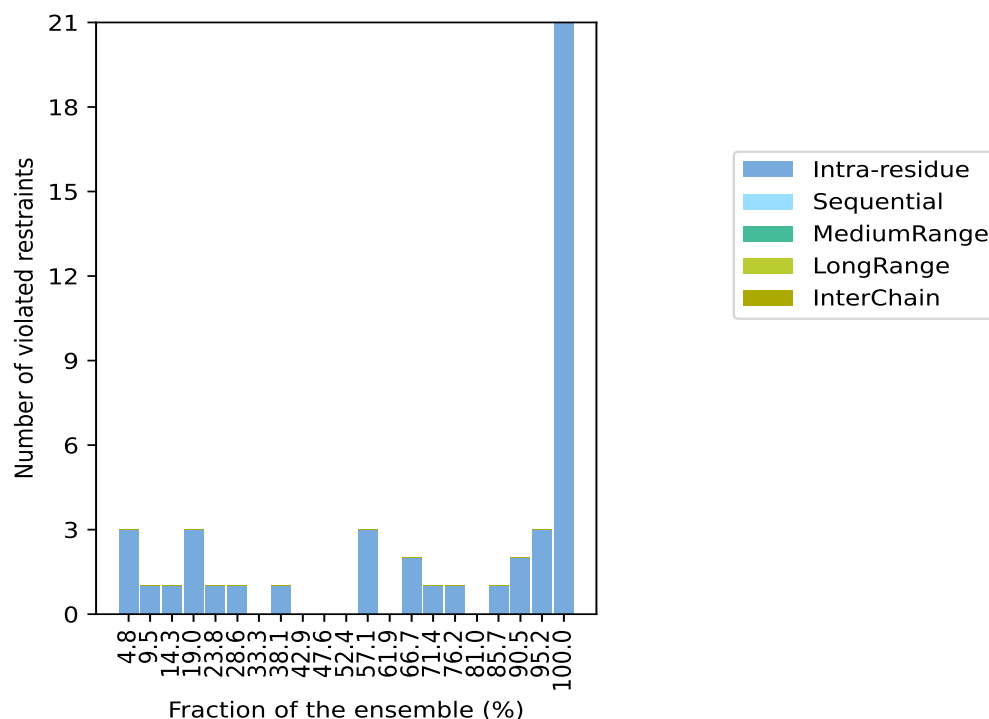
9.3 Distance violation statistics for the ensemble

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, 2333(IR:677, SQ:562, MR:336, LR:698, IC:60) 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 | % |
| 3 | 0 | 0 | 0 | 0 | 3 | 1 | 4.8 |
| 1 | 0 | 0 | 0 | 0 | 1 | 2 | 9.5 |
| 1 | 0 | 0 | 0 | 0 | 1 | 3 | 14.3 |
| 3 | 0 | 0 | 0 | 0 | 3 | 4 | 19.0 |
| 1 | 0 | 0 | 0 | 0 | 1 | 5 | 23.8 |
| 1 | 0 | 0 | 0 | 0 | 1 | 6 | 28.6 |
| 0 | 0 | 0 | 0 | 0 | 0 | 7 | 33.3 |
| 1 | 0 | 0 | 0 | 0 | 1 | 8 | 38.1 |
| 0 | 0 | 0 | 0 | 0 | 0 | 9 | 42.9 |
| 0 | 0 | 0 | 0 | 0 | 0 | 10 | 47.6 |
| 0 | 0 | 0 | 0 | 0 | 0 | 11 | 52.4 |
| 3 | 0 | 0 | 0 | 0 | 3 | 12 | 57.1 |
| 0 | 0 | 0 | 0 | 0 | 0 | 13 | 61.9 |
| 2 | 0 | 0 | 0 | 0 | 2 | 14 | 66.7 |
| 1 | 0 | 0 | 0 | 0 | 1 | 15 | 71.4 |
| 1 | 0 | 0 | 0 | 0 | 1 | 16 | 76.2 |
| 0 | 0 | 0 | 0 | 0 | 0 | 17 | 81.0 |
| 1 | 0 | 0 | 0 | 0 | 1 | 18 | 85.7 |
| 2 | 0 | 0 | 0 | 0 | 2 | 19 | 90.5 |
| 3 | 0 | 0 | 0 | 0 | 3 | 20 | 95.2 |
| 21 | 0 | 0 | 0 | 0 | 21 | 21 | 100.0 |

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

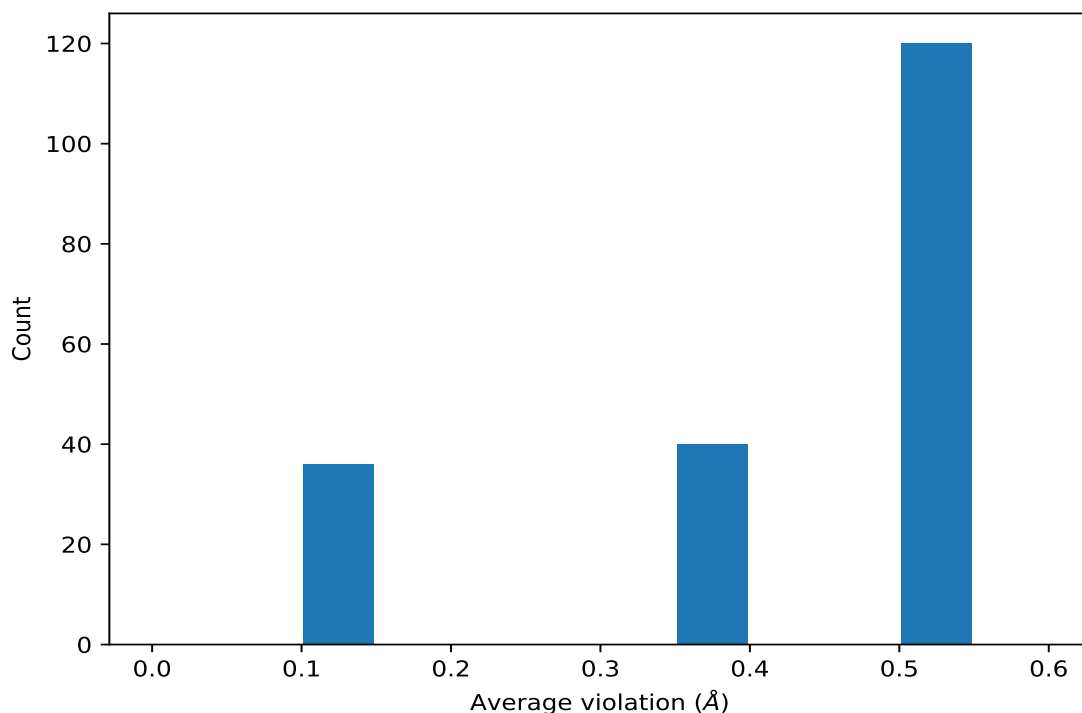
9.3.1 Bar graph : Distance violation statistics for the ensemble [\(i\)](#)



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) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 21 | 0.53 | 0.01 | 0.53 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 21 | 0.53 | 0.01 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 21 | 0.53 | 0.01 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 21 | 0.53 | 0.0 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 21 | 0.53 | 0.0 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 21 | 0.53 | 0.0 | 0.53 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 21 | 0.36 | 0.01 | 0.36 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 21 | 0.12 | 0.0 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 21 | 0.12 | 0.0 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 21 | 0.12 | 0.0 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 21 | 0.12 | 0.0 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 21 | 0.12 | 0.0 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 21 | 0.12 | 0.0 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 21 | 0.12 | 0.0 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 21 | 0.11 | 0.0 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 21 | 0.11 | 0.0 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 21 | 0.11 | 0.0 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 21 | 0.11 | 0.0 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 21 | 0.11 | 0.0 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 21 | 0.11 | 0.0 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 21 | 0.11 | 0.0 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 21 | 0.11 | 0.0 | 0.11 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 20 | 0.12 | 0.0 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 20 | 0.12 | 0.0 | 0.12 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 20 | 0.11 | 0.0 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 19 | 0.11 | 0.0 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 19 | 0.11 | 0.0 | 0.11 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 18 | 0.12 | 0.0 | 0.12 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 16 | 0.11 | 0.0 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 15 | 0.11 | 0.0 | 0.11 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 14 | 0.12 | 0.0 | 0.12 |

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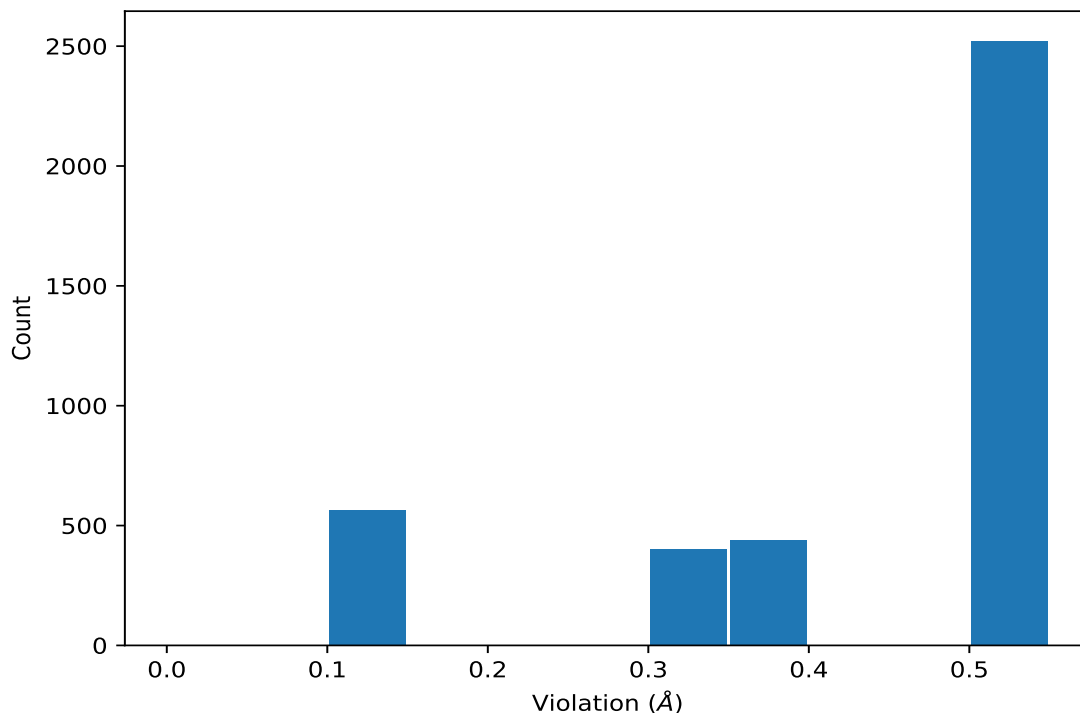
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|--------------|---------------|---------------------|----------|---------------------|------------|
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 14 | 0.11 | 0.0 | 0.11 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 12 | 0.12 | 0.0 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 12 | 0.12 | 0.0 | 0.12 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 12 | 0.11 | 0.0 | 0.11 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 8 | 0.12 | 0.0 | 0.12 |
| (1,2119) | 1:B:31:SER:H | 1:B:31:SER:HA | 6 | 0.11 | 0.0 | 0.11 |
| (1,1024) | 1:A:50:MET:H | 1:A:50:MET:HA | 5 | 0.12 | 0.0 | 0.12 |
| (1,810) | 1:A:2:VAL:H | 1:A:2:VAL:HA | 4 | 0.12 | 0.0 | 0.12 |
| (1,1021) | 1:A:49:GLU:H | 1:A:49:GLU:HA | 4 | 0.12 | 0.0 | 0.12 |
| (1,2180) | 1:B:49:GLU:H | 1:B:49:GLU:HA | 4 | 0.12 | 0.0 | 0.12 |
| (1,2005) | 1:B:7:GLU:H | 1:B:7:GLU:HA | 3 | 0.11 | 0.0 | 0.11 |
| (1,994) | 1:A:43:ILE:H | 1:A:43:ILE:HA | 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) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 7 | 0.55 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 7 | 0.55 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 15 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 15 | 0.55 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 15 | 0.55 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 1 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 1 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 2 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 11 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 11 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 16 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 16 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 18 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 18 | 0.54 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 18 | 0.54 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 1 | 0.54 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 3 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 3 | 0.54 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 3 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 4 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 4 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 5 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 18 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 18 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 20 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 20 | 0.54 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 20 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 6 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 6 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 8 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 10 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 10 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 11 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 11 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 16 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 17 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 17 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 19 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 19 | 0.54 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 19 | 0.54 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 3 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 3 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 4 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 5 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 5 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 6 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 6 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 8 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 9 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 9 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 10 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 10 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 12 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 12 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 13 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 14 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 14 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 15 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 15 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 17 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 19 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 19 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 20 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 20 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:H | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HA | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD23 | 21 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD21 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD22 | 21 | 0.53 |
| (1,802) | 1:A:1:LEU:HG | 1:A:1:LEU:HD23 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 2 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 4 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 4 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 5 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 5 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 6 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 7 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 7 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 8 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 8 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 9 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 9 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 10 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 11 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 11 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 12 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 12 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 13 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 14 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 14 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 16 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 16 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 17 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 17 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 18 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 19 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 19 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 20 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 20 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:H | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HA | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD11 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD12 | 21 | 0.53 |
| (1,801) | 1:A:1:LEU:HG | 1:A:1:LEU:HD13 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 1 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 1 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 2 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 2 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 3 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 3 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 6 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 7 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 7 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 8 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 8 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 9 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 10 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 10 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 11 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 11 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 12 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 12 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 13 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 14 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 14 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 15 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 15 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 16 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 17 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 17 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 19 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 19 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:H | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HA | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD23 | 21 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD21 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD22 | 21 | 0.53 |
| (1,1961) | 1:B:1:LEU:HG | 1:B:1:LEU:HD23 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 1 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 2 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 2 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 3 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 3 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 4 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 5 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 5 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 7 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 7 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 9 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 9 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 12 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 13 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 13 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 14 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 14 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 15 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 18 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 18 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 20 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 20 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:H | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HA | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD11 | 21 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD11 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD12 | 21 | 0.53 |
| (1,1960) | 1:B:1:LEU:HG | 1:B:1:LEU:HD13 | 21 | 0.53 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 8 | 0.38 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 20 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 20 | 0.38 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 20 | 0.38 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 3 | 0.38 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 3 | 0.38 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 1 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 1 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 2 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 5 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 6 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 6 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 7 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 11 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 11 | 0.37 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 11 | 0.37 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 6 | 0.37 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 12 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 12 | 0.37 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 13 | 0.37 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 21 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 21 | 0.37 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 21 | 0.37 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 10 | 0.36 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 14 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 14 | 0.36 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 15 | 0.36 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 15 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 1 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 1 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 4 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 5 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 5 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 11 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 17 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 17 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 20 | 0.36 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 20 | 0.36 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 9 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 9 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 13 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 16 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 16 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 19 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 21 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 21 | 0.35 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 21 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 2 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 7 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 7 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 8 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 10 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 10 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 14 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 16 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 16 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 18 | 0.35 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 18 | 0.35 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 4 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 4 | 0.34 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 17 | 0.34 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 17 | 0.34 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 9 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 9 | 0.34 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 15 | 0.34 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:H | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HA | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HB2 | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HB3 | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD11 | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD12 | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD13 | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB2 | 19 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1959) | 1:B:1:LEU:HD21 | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD22 | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HD23 | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB2 | 19 | 0.34 |
| (1,1959) | 1:B:1:LEU:HG | 1:B:1:LEU:HB3 | 19 | 0.34 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 3 | 0.33 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:H | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HA | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HB2 | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HB3 | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD11 | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD12 | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD13 | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD21 | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB2 | 12 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,800) | 1:A:1:LEU:HD22 | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HD23 | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB2 | 12 | 0.33 |
| (1,800) | 1:A:1:LEU:HG | 1:A:1:LEU:HB3 | 12 | 0.33 |
| (1,994) | 1:A:43:ILE:H | 1:A:43:ILE:HA | 14 | 0.12 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 10 | 0.12 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 14 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 1 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 2 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 3 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 4 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 5 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 6 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 7 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 8 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 9 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 10 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 11 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 12 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 13 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 14 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 15 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 16 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 17 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 18 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 19 | 0.12 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 21 | 0.12 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 4 | 0.12 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 9 | 0.12 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 14 | 0.12 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 17 | 0.12 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 18 | 0.12 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 20 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 1 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 2 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 3 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 5 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 6 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 7 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 8 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 9 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 10 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 12 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 14 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 16 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 18 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 19 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 20 | 0.12 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 21 | 0.12 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 7 | 0.12 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 14 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 1 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 3 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 4 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 5 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 6 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 9 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 10 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 11 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 12 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 13 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 14 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 15 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 16 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 17 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 20 | 0.12 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 21 | 0.12 |
| (1,810) | 1:A:2:VAL:H | 1:A:2:VAL:HA | 2 | 0.12 |
| (1,810) | 1:A:2:VAL:H | 1:A:2:VAL:HA | 13 | 0.12 |
| (1,810) | 1:A:2:VAL:H | 1:A:2:VAL:HA | 17 | 0.12 |
| (1,810) | 1:A:2:VAL:H | 1:A:2:VAL:HA | 19 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 1 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 2 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 3 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 4 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 5 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 6 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 7 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 8 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 9 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 10 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 11 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 12 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 13 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 14 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 15 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 16 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 17 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 18 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 19 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 20 | 0.12 |
| (1,2285) | 1:B:72:VAL:H | 1:B:72:VAL:HA | 21 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 1 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 6 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 7 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 10 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 14 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 15 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 16 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 17 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 18 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 19 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 20 | 0.12 |
| (1,2183) | 1:B:50:MET:H | 1:B:50:MET:HA | 21 | 0.12 |
| (1,2180) | 1:B:49:GLU:H | 1:B:49:GLU:HA | 4 | 0.12 |
| (1,2180) | 1:B:49:GLU:H | 1:B:49:GLU:HA | 11 | 0.12 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 11 | 0.12 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 20 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 1 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 2 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 3 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 4 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 5 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 6 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 7 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 8 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 9 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 10 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 11 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 12 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 13 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 14 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 15 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 16 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 18 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 19 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 20 | 0.12 |
| (1,2170) | 1:B:47:THR:H | 1:B:47:THR:HA | 21 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 1 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 2 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 3 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 6 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 7 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 8 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 9 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 10 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 11 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 12 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 13 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 14 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 15 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 17 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 18 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 19 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 20 | 0.12 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 21 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 2 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 3 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 6 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 7 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 8 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 9 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 10 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 11 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 13 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 15 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 16 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 17 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 18 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 19 | 0.12 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 21 | 0.12 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 3 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 5 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 6 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 11 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 13 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 16 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 18 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 19 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 20 | 0.12 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 21 | 0.12 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 1 | 0.12 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 10 | 0.12 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 13 | 0.12 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 15 | 0.12 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 17 | 0.12 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 18 | 0.12 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 19 | 0.12 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 21 | 0.12 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 3 | 0.12 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 11 | 0.12 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 12 | 0.12 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 16 | 0.12 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 17 | 0.12 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 20 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 1 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 2 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 3 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 6 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 7 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 8 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 9 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 12 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 13 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 15 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 16 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 18 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 19 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 20 | 0.12 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 21 | 0.12 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 2 | 0.12 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 5 | 0.12 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 6 | 0.12 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 9 | 0.12 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 13 | 0.12 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 20 | 0.12 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 9 | 0.12 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 11 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 14 | 0.12 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 15 | 0.12 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 17 | 0.12 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 18 | 0.12 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 19 | 0.12 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 2 | 0.12 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 3 | 0.12 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 4 | 0.12 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 7 | 0.12 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 8 | 0.12 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 12 | 0.12 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 16 | 0.12 |
| (1,1969) | 1:B:2:VAL:H | 1:B:2:VAL:HA | 17 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 1 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 2 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 3 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 4 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 5 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 6 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 7 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 8 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 9 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 10 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 11 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 12 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 13 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 14 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 15 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 16 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 17 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 18 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 19 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 20 | 0.12 |
| (1,1126) | 1:A:72:VAL:H | 1:A:72:VAL:HA | 21 | 0.12 |
| (1,1024) | 1:A:50:MET:H | 1:A:50:MET:HA | 2 | 0.12 |
| (1,1024) | 1:A:50:MET:H | 1:A:50:MET:HA | 3 | 0.12 |
| (1,1024) | 1:A:50:MET:H | 1:A:50:MET:HA | 5 | 0.12 |
| (1,1024) | 1:A:50:MET:H | 1:A:50:MET:HA | 16 | 0.12 |
| (1,1024) | 1:A:50:MET:H | 1:A:50:MET:HA | 17 | 0.12 |
| (1,1021) | 1:A:49:GLU:H | 1:A:49:GLU:HA | 13 | 0.12 |
| (1,1021) | 1:A:49:GLU:H | 1:A:49:GLU:HA | 18 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 3 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 5 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 7 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 8 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 9 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 11 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 12 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 14 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 16 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 18 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 19 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 20 | 0.12 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 21 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 2 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 3 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 5 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 10 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 11 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 13 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 14 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 16 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 18 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 19 | 0.12 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 20 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 1 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 2 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 3 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 5 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 10 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 11 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 12 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 13 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 14 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 16 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 18 | 0.12 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 21 | 0.12 |
| (1,994) | 1:A:43:ILE:H | 1:A:43:ILE:HA | 16 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 1 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 2 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 3 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 4 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 6 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 7 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 8 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 9 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 10 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 11 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 12 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 13 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 14 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 15 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 16 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 17 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 18 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 19 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 20 | 0.11 |
| (1,985) | 1:A:41:VAL:H | 1:A:41:VAL:HA | 21 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 1 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 2 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 3 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 4 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 5 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 6 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 7 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 8 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 9 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 11 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 12 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 13 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 15 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 16 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 17 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 18 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 19 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 20 | 0.11 |
| (1,977) | 1:A:35:THR:H | 1:A:35:THR:HA | 21 | 0.11 |
| (1,969) | 1:A:34:VAL:H | 1:A:34:VAL:HA | 20 | 0.11 |
| (1,851) | 1:A:8:ALA:H | 1:A:8:ALA:HA | 9 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 1 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 2 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 3 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 5 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 7 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 8 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 10 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 11 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 12 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 13 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 16 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 19 | 0.11 |
| (1,837) | 1:A:6:VAL:H | 1:A:6:VAL:HA | 21 | 0.11 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 4 | 0.11 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 11 | 0.11 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 13 | 0.11 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 15 | 0.11 |
| (1,832) | 1:A:5:GLN:H | 1:A:5:GLN:HA | 17 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 1 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 2 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 3 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 4 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 8 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 9 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 10 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 11 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 12 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 13 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 15 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 18 | 0.11 |
| (1,822) | 1:A:4:ILE:H | 1:A:4:ILE:HA | 21 | 0.11 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 2 | 0.11 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 7 | 0.11 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 8 | 0.11 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 18 | 0.11 |
| (1,819) | 1:A:3:ALA:H | 1:A:3:ALA:HA | 19 | 0.11 |
| (1,2303) | 1:B:75:VAL:H | 1:B:75:VAL:HA | 4 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 1 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 2 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 3 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 4 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 5 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 6 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 7 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 8 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 10 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 11 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 12 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 13 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 14 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 15 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 16 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 17 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 18 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 19 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 20 | 0.11 |
| (1,2294) | 1:B:73:TYR:H | 1:B:73:TYR:HA | 21 | 0.11 |
| (1,2180) | 1:B:49:GLU:H | 1:B:49:GLU:HA | 2 | 0.11 |
| (1,2180) | 1:B:49:GLU:H | 1:B:49:GLU:HA | 5 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 3 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 4 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 5 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 7 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 8 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 10 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 12 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 14 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 16 | 0.11 |
| (1,2176) | 1:B:48:PHE:H | 1:B:48:PHE:HA | 21 | 0.11 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 5 | 0.11 |
| (1,2168) | 1:B:46:PHE:H | 1:B:46:PHE:HA | 16 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 2 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 3 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 4 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 5 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 7 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 8 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 9 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 10 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 11 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 12 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 13 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 15 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 18 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 19 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 20 | 0.11 |
| (1,2163) | 1:B:45:ARG:H | 1:B:45:ARG:HA | 21 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 1 | 0.11 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 4 | 0.11 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 5 | 0.11 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 14 | 0.11 |
| (1,2153) | 1:B:43:ILE:H | 1:B:43:ILE:HA | 20 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 1 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 2 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 3 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 4 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 5 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 6 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 7 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 8 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 9 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 10 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 11 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 12 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 13 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 14 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 15 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 16 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 17 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 18 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 19 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 20 | 0.11 |
| (1,2144) | 1:B:41:VAL:H | 1:B:41:VAL:HA | 21 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 1 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 2 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 4 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 5 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 6 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 7 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 8 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 9 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 10 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 11 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 12 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 13 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 14 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 15 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 16 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 17 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 18 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 19 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 20 | 0.11 |
| (1,2136) | 1:B:35:THR:H | 1:B:35:THR:HA | 21 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 1 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 2 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 3 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 4 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 7 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 8 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 9 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 10 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 12 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 14 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 15 | 0.11 |
| (1,2128) | 1:B:34:VAL:H | 1:B:34:VAL:HA | 17 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 2 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 3 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 4 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 5 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 6 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 7 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 8 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 9 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 11 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 12 | 0.11 |
| (1,2122) | 1:B:32:ALA:H | 1:B:32:ALA:HA | 16 | 0.11 |
| (1,2119) | 1:B:31:SER:H | 1:B:31:SER:HA | 2 | 0.11 |
| (1,2119) | 1:B:31:SER:H | 1:B:31:SER:HA | 3 | 0.11 |
| (1,2119) | 1:B:31:SER:H | 1:B:31:SER:HA | 5 | 0.11 |
| (1,2119) | 1:B:31:SER:H | 1:B:31:SER:HA | 8 | 0.11 |
| (1,2119) | 1:B:31:SER:H | 1:B:31:SER:HA | 11 | 0.11 |
| (1,2119) | 1:B:31:SER:H | 1:B:31:SER:HA | 12 | 0.11 |
| (1,2005) | 1:B:7:GLU:H | 1:B:7:GLU:HA | 2 | 0.11 |
| (1,2005) | 1:B:7:GLU:H | 1:B:7:GLU:HA | 8 | 0.11 |
| (1,2005) | 1:B:7:GLU:H | 1:B:7:GLU:HA | 12 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 1 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 2 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 4 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 5 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 6 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 8 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 9 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 10 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 13 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 14 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 15 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 18 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 19 | 0.11 |
| (1,1996) | 1:B:6:VAL:H | 1:B:6:VAL:HA | 21 | 0.11 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 4 | 0.11 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 5 | 0.11 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 10 | 0.11 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 11 | 0.11 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 14 | 0.11 |
| (1,1991) | 1:B:5:GLN:H | 1:B:5:GLN:HA | 17 | 0.11 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 3 | 0.11 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 4 | 0.11 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 7 | 0.11 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 8 | 0.11 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 10 | 0.11 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 12 | 0.11 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 15 | 0.11 |
| (1,1981) | 1:B:4:ILE:H | 1:B:4:ILE:HA | 19 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 1 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 2 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 3 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 4 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 5 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 7 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 8 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 10 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 13 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 16 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 20 | 0.11 |
| (1,1978) | 1:B:3:ALA:H | 1:B:3:ALA:HA | 21 | 0.11 |
| (1,1144) | 1:A:75:VAL:H | 1:A:75:VAL:HA | 8 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 1 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 2 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 3 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 4 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 5 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 7 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 8 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 9 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 10 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 11 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 12 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 13 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 14 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 15 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 16 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 17 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 18 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 19 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 20 | 0.11 |
| (1,1135) | 1:A:73:TYR:H | 1:A:73:TYR:HA | 21 | 0.11 |
| (1,1021) | 1:A:49:GLU:H | 1:A:49:GLU:HA | 19 | 0.11 |
| (1,1021) | 1:A:49:GLU:H | 1:A:49:GLU:HA | 21 | 0.11 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 4 | 0.11 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 13 | 0.11 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 15 | 0.11 |
| (1,1011) | 1:A:47:THR:H | 1:A:47:THR:HA | 17 | 0.11 |
| (1,1009) | 1:A:46:PHE:H | 1:A:46:PHE:HA | 17 | 0.11 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 7 | 0.11 |
| (1,1004) | 1:A:45:ARG:H | 1:A:45:ARG:HA | 8 | 0.11 |

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

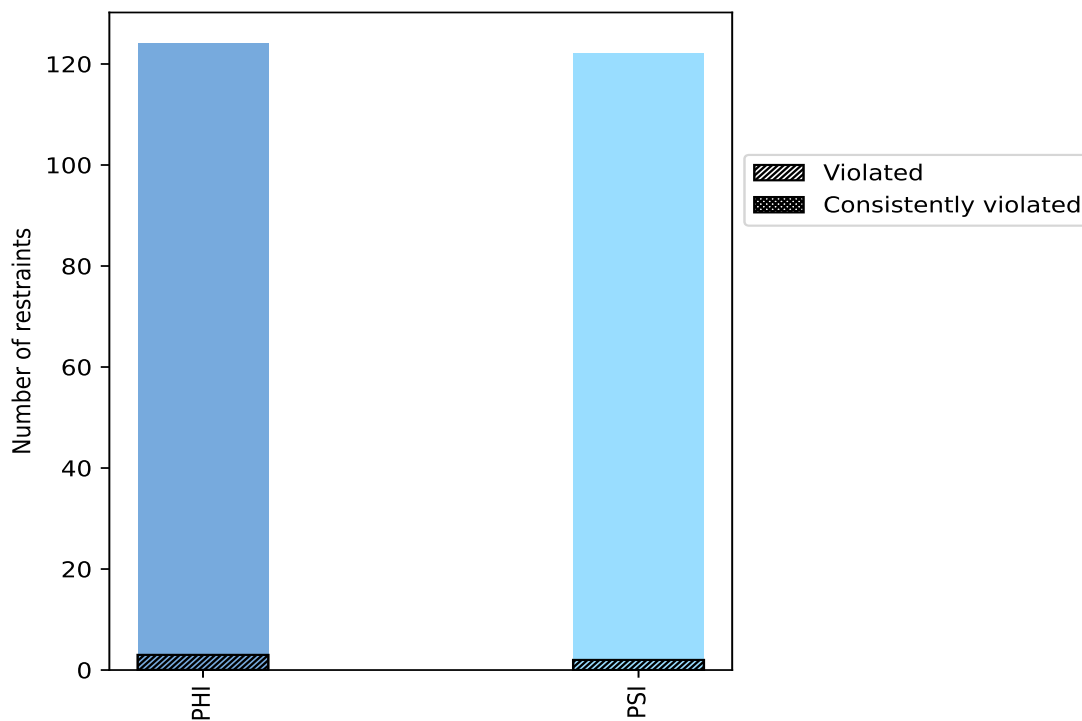
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PHI | 124 | 50.4 | 3 | 2.4 | 1.2 | 0 | 0.0 | 0.0 |
| PSI | 122 | 49.6 | 2 | 1.6 | 0.8 | 0 | 0.0 | 0.0 |
| Total | 246 | 100.0 | 5 | 2.0 | 2.0 | 0 | 0.0 | 0.0 |

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

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



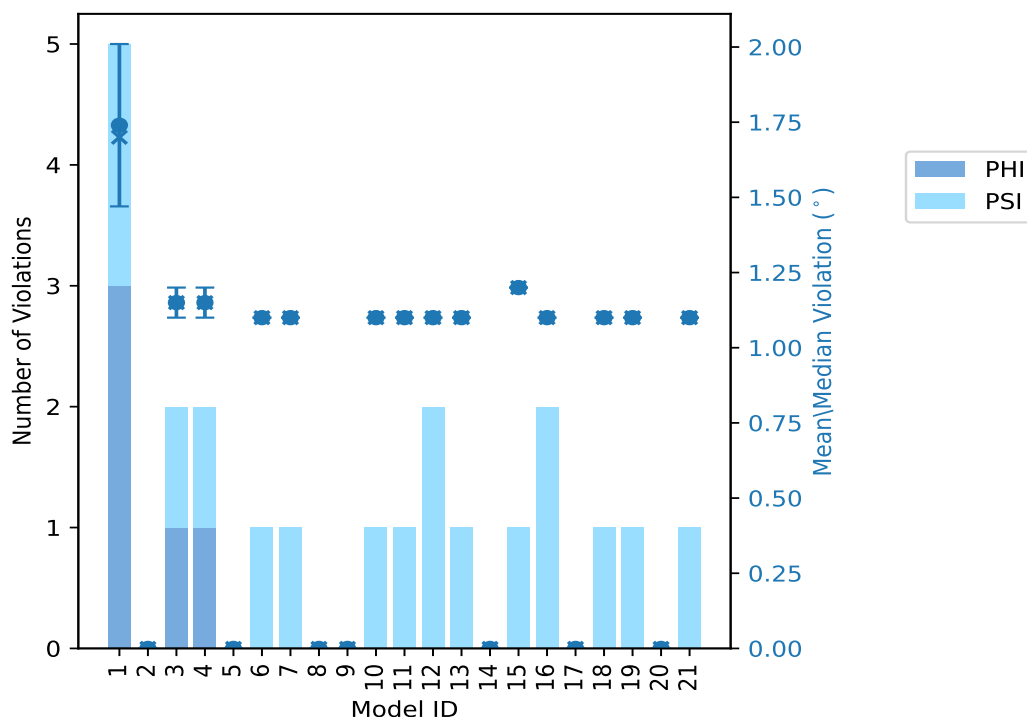
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PHI | PSI | Total | | | | |
| 1 | 3 | 2 | 5 | 1.74 | 2.1 | 0.27 | 1.7 |
| 2 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 3 | 1 | 1 | 2 | 1.15 | 1.2 | 0.05 | 1.15 |
| 4 | 1 | 1 | 2 | 1.15 | 1.2 | 0.05 | 1.15 |
| 5 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 6 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 7 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 8 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 9 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 10 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 11 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 12 | 0 | 2 | 2 | 1.1 | 1.1 | 0.0 | 1.1 |
| 13 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 14 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 15 | 0 | 1 | 1 | 1.2 | 1.2 | 0.0 | 1.2 |
| 16 | 0 | 2 | 2 | 1.1 | 1.1 | 0.0 | 1.1 |
| 17 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 18 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 19 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 20 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 21 | 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 | |
|-------------------------------|-----|-------|--------------------------|------|
| PHI | PSI | Total | Count ¹ | % |
| 1 | 0 | 1 | 1 | 4.8 |
| 2 | 0 | 2 | 2 | 9.5 |
| 0 | 0 | 0 | 3 | 14.3 |
| 0 | 0 | 0 | 4 | 19.0 |
| 0 | 0 | 0 | 5 | 23.8 |
| 0 | 1 | 1 | 6 | 28.6 |
| 0 | 0 | 0 | 7 | 33.3 |
| 0 | 0 | 0 | 8 | 38.1 |
| 0 | 0 | 0 | 9 | 42.9 |
| 0 | 0 | 0 | 10 | 47.6 |
| 0 | 1 | 1 | 11 | 52.4 |

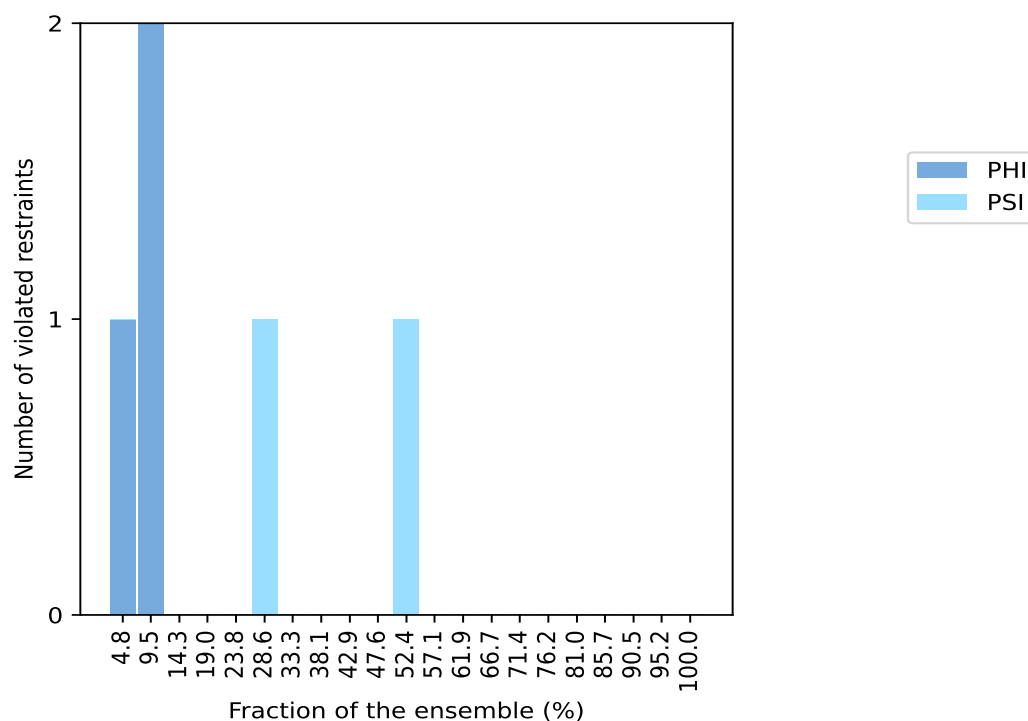
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI | PSI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 57.1 |
| 0 | 0 | 0 | 13 | 61.9 |
| 0 | 0 | 0 | 14 | 66.7 |
| 0 | 0 | 0 | 15 | 71.4 |
| 0 | 0 | 0 | 16 | 76.2 |
| 0 | 0 | 0 | 17 | 81.0 |
| 0 | 0 | 0 | 18 | 85.7 |
| 0 | 0 | 0 | 19 | 90.5 |
| 0 | 0 | 0 | 20 | 95.2 |
| 0 | 0 | 0 | 21 | 100.0 |

¹ Number of models with violations

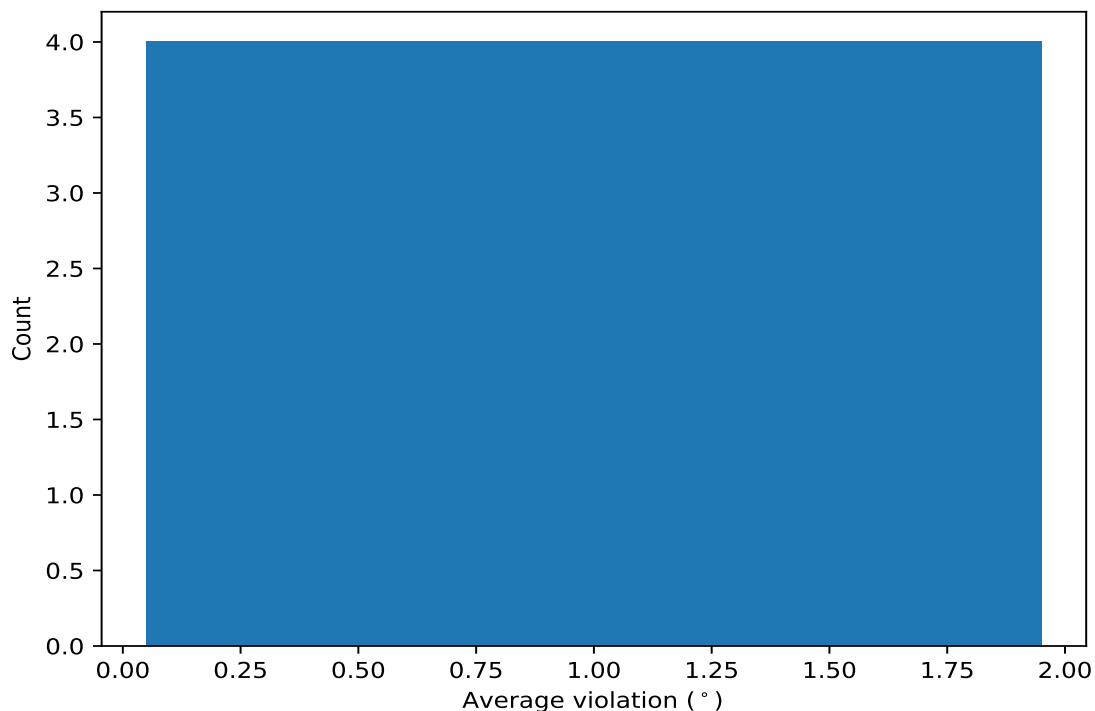
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

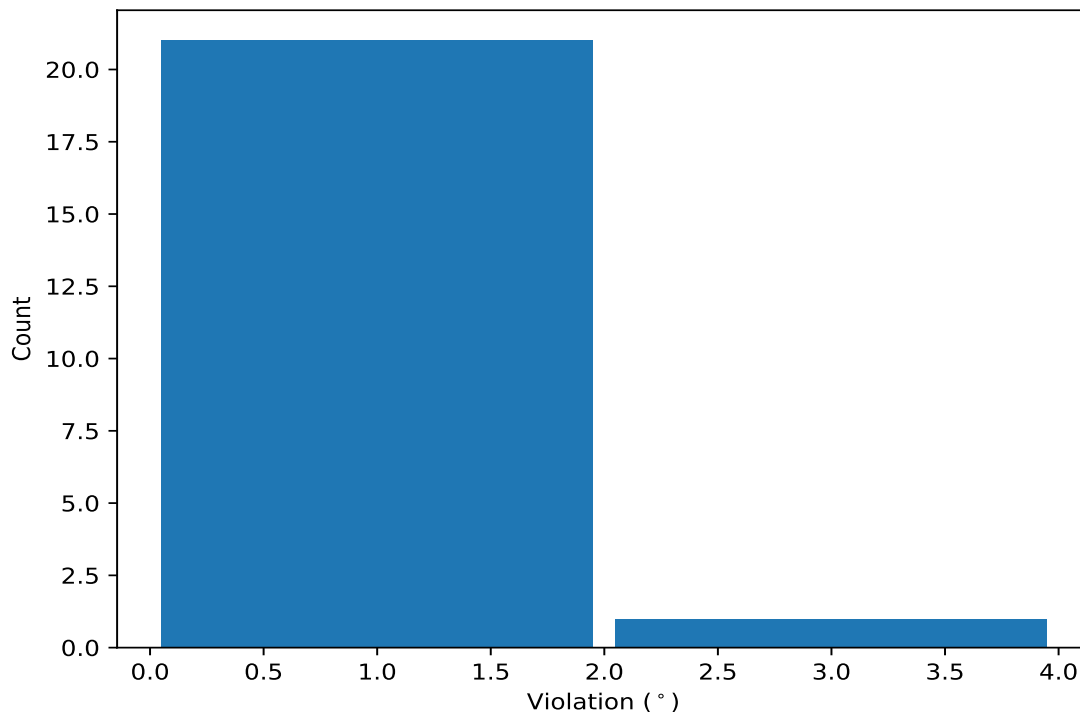
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 11 | 1.15 | 0.17 | 1.1 |
| (1,229) | 1:B:66:VAL:N | 1:B:66:VAL:CA | 1:B:66:VAL:C | 1:B:67:GLU:N | 6 | 1.23 | 0.21 | 1.15 |
| (1,83) | 1:A:54:LYS:C | 1:A:55:HIS:N | 1:A:55:HIS:CA | 1:A:55:HIS:C | 2 | 1.6 | 0.5 | 1.6 |
| (1,206) | 1:B:54:LYS:C | 1:B:55:HIS:N | 1:B:55:HIS:CA | 1:B:55:HIS:C | 2 | 1.55 | 0.35 | 1.55 |

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 (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,83) | 1:A:54:LYS:C | 1:A:55:HIS:N | 1:A:55:HIS:CA | 1:A:55:HIS:C | 1 | 2.1 |
| (1,206) | 1:B:54:LYS:C | 1:B:55:HIS:N | 1:B:55:HIS:CA | 1:B:55:HIS:C | 1 | 1.9 |
| (1,229) | 1:B:66:VAL:N | 1:B:66:VAL:CA | 1:B:66:VAL:C | 1:B:67:GLU:N | 1 | 1.7 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 1 | 1.7 |
| (1,198) | 1:B:48:PHE:C | 1:B:49:GLU:N | 1:B:49:GLU:CA | 1:B:49:GLU:C | 1 | 1.3 |
| (1,229) | 1:B:66:VAL:N | 1:B:66:VAL:CA | 1:B:66:VAL:C | 1:B:67:GLU:N | 3 | 1.2 |
| (1,229) | 1:B:66:VAL:N | 1:B:66:VAL:CA | 1:B:66:VAL:C | 1:B:67:GLU:N | 15 | 1.2 |
| (1,206) | 1:B:54:LYS:C | 1:B:55:HIS:N | 1:B:55:HIS:CA | 1:B:55:HIS:C | 4 | 1.2 |
| (1,83) | 1:A:54:LYS:C | 1:A:55:HIS:N | 1:A:55:HIS:CA | 1:A:55:HIS:C | 3 | 1.1 |
| (1,229) | 1:B:66:VAL:N | 1:B:66:VAL:CA | 1:B:66:VAL:C | 1:B:67:GLU:N | 12 | 1.1 |
| (1,229) | 1:B:66:VAL:N | 1:B:66:VAL:CA | 1:B:66:VAL:C | 1:B:67:GLU:N | 16 | 1.1 |
| (1,229) | 1:B:66:VAL:N | 1:B:66:VAL:CA | 1:B:66:VAL:C | 1:B:67:GLU:N | 21 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 4 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 6 | 1.1 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|------------|---------------|---------------|---------------|---------------|-----------------|----------------------|
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 7 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 10 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 11 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 12 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 13 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 16 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 18 | 1.1 |
| (1,106) | 1:A:66:VAL:N | 1:A:66:VAL:CA | 1:A:66:VAL:C | 1:A:67:GLU:N | 19 | 1.1 |