



Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 09:03 AM EDT

PDB ID : 2LBF
Title : Solution structure of the dimerization domain of human ribosomal protein P1/P2 heterodimer
Authors : Lee, K.-M.; Yu, C.W.-H.; Chiu, T.Y.-H.; Sze, K.-H.; Shaw, P.-C.; Wong, K.-B.
Deposited on : 2011-03-30

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

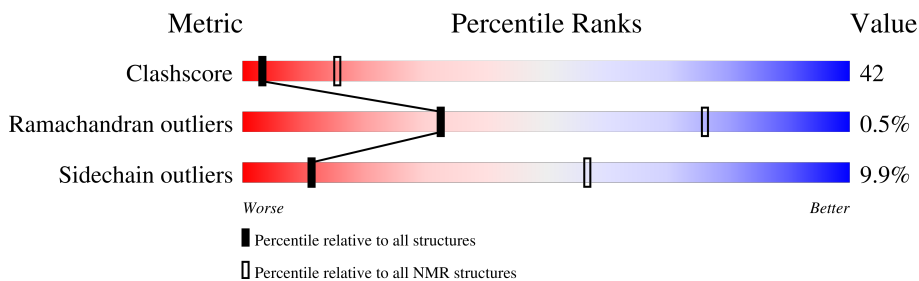
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 69%.

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 | 69 | |
| 2 | B | 70 | |

2 Ensemble composition and analysis

This entry contains 10 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|--------------------------------------|--------------------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:3-A:60, B:103-B:160 (116) | 0.33 | 9 |

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 2 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2031 atoms, of which 1029 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 60S acidic ribosomal protein P1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| | | | Total | C | H | N | O | S | |
| 1 | A | 69 | 1002 | 318 | 505 | 80 | 96 | 3 | 0 |

- Molecule 2 is a protein called 60S acidic ribosomal protein P2.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|-------|
| | | | Total | C | H | N | O | S | |
| 2 | B | 70 | 1029 | 314 | 524 | 87 | 103 | 1 | 0 |

There is a discrepancy between the modelled and reference sequences:

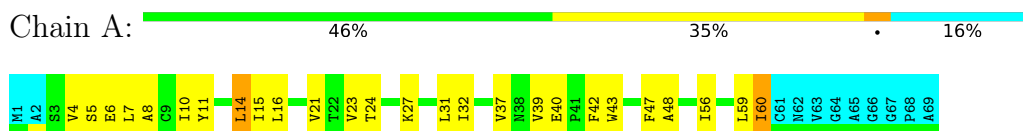
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 100 | ALA | - | expression tag | UNP P05387 |

4 Residue-property plots

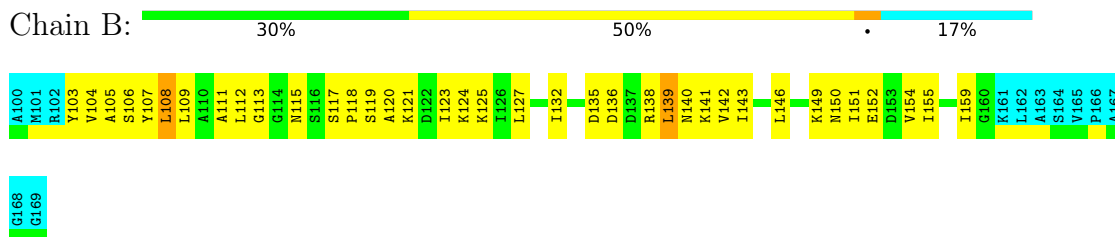
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2

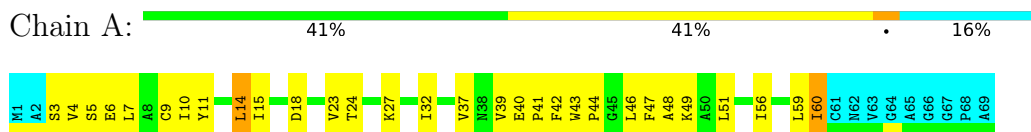


4.2 Scores per residue for each member of the ensemble

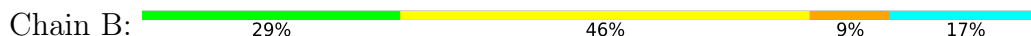
Colouring as in section 4.1 above.

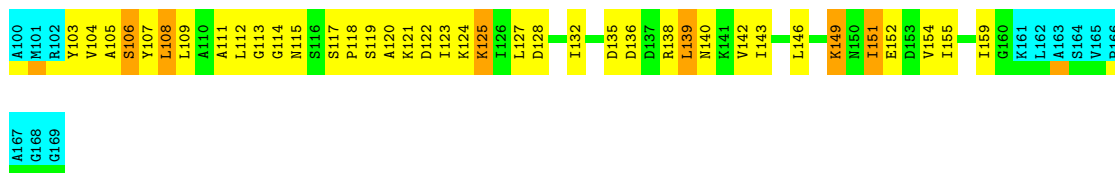
4.2.1 Score per residue for model 1

- Molecule 1: 60S acidic ribosomal protein P1



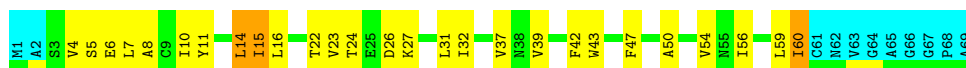
- Molecule 2: 60S acidic ribosomal protein P2





4.2.2 Score per residue for model 2

- Molecule 1: 60S acidic ribosomal protein P1

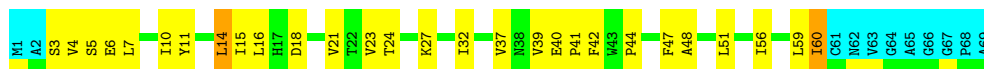


- Molecule 2: 60S acidic ribosomal protein P2

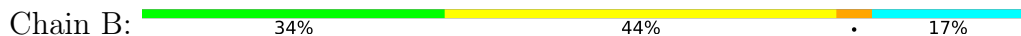


4.2.3 Score per residue for model 3

- Molecule 1: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2



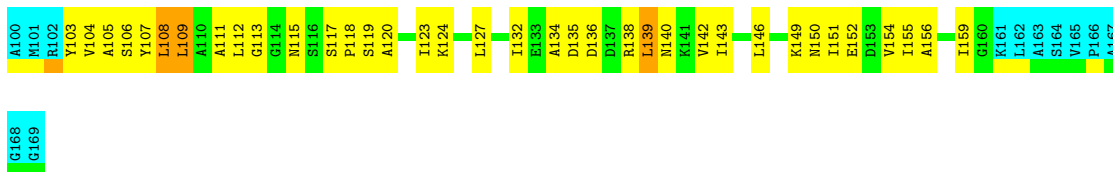
4.2.4 Score per residue for model 4

- Molecule 1: 60S acidic ribosomal protein P1





- Molecule 2: 60S acidic ribosomal protein P2

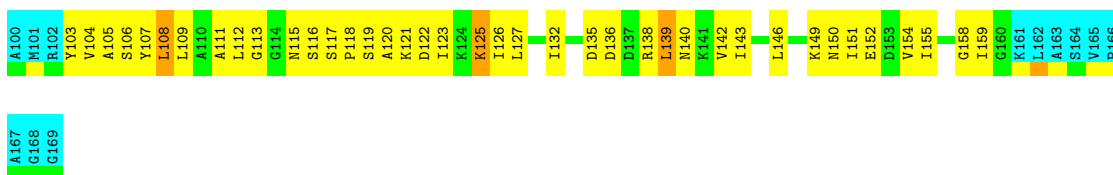
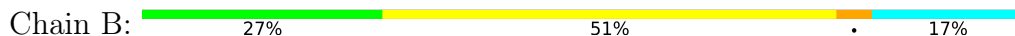


4.2.5 Score per residue for model 5

- Molecule 1: 60S acidic ribosomal protein P1

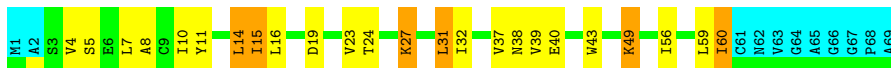


- Molecule 2: 60S acidic ribosomal protein P2

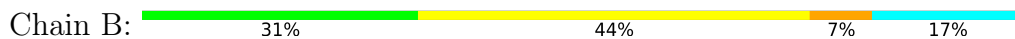


4.2.6 Score per residue for model 6

- Molecule 1: 60S acidic ribosomal protein P1



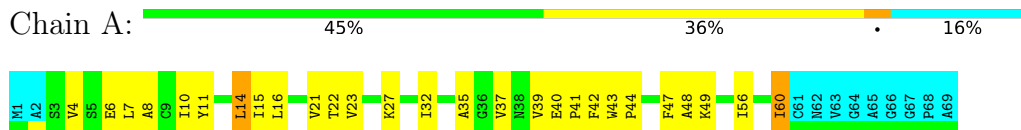
- Molecule 2: 60S acidic ribosomal protein P2



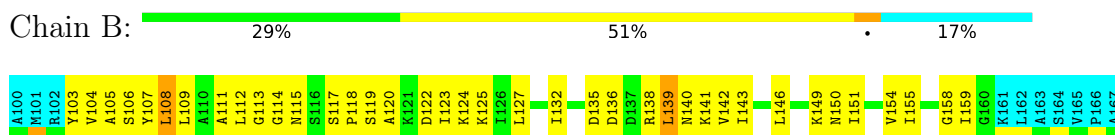
G169

4.2.7 Score per residue for model 7

- Molecule 1: 60S acidic ribosomal protein P1

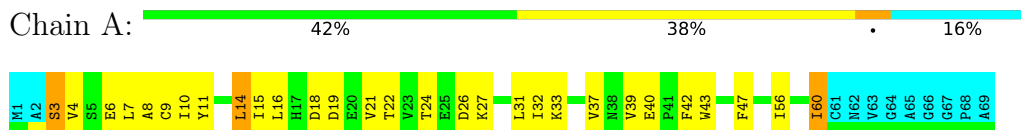


- Molecule 2: 60S acidic ribosomal protein P2

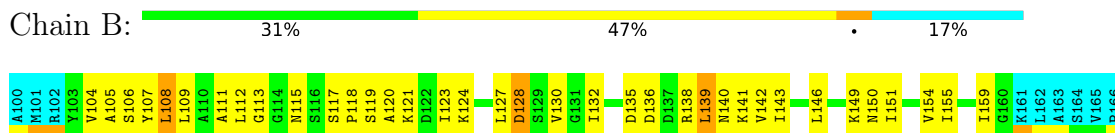
G168
G169

4.2.8 Score per residue for model 8

- Molecule 1: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2

A167
G168
G169

4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: 60S acidic ribosomal protein P1



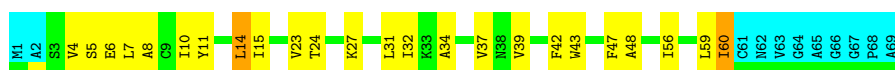


- Molecule 2: 60S acidic ribosomal protein P2



4.2.10 Score per residue for model 10

- Molecule 1: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

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

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

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1202 |
| Number of shifts mapped to atoms | 1202 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 69% |

6 Model quality

6.1 Standard geometry

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

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 | 433 | 443 | 442 | 31±2 |
| 2 | B | 425 | 434 | 434 | 55±4 |
| All | All | 8580 | 8770 | 8760 | 721 |

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 42.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:136:ASP:HA | 2:B:139:LEU:HD11 | 0.90 | 1.36 | 6 | 10 |
| 1:A:37:VAL:HB | 2:B:113:GLY:HA3 | 0.88 | 1.43 | 1 | 2 |
| 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 0.81 | 1.51 | 1 | 7 |
| 1:A:4:VAL:HG13 | 2:B:112:LEU:HG | 0.80 | 1.53 | 2 | 10 |
| 2:B:124:LYS:HD2 | 2:B:127:LEU:HD11 | 0.80 | 1.53 | 6 | 2 |
| 1:A:37:VAL:HB | 2:B:113:GLY:HA2 | 0.80 | 1.52 | 7 | 8 |
| 2:B:139:LEU:O | 2:B:143:ILE:HG12 | 0.79 | 1.76 | 6 | 6 |
| 1:A:7:LEU:HD12 | 1:A:10:ILE:HD12 | 0.75 | 1.57 | 9 | 10 |
| 2:B:127:LEU:HB2 | 2:B:132:ILE:HB | 0.73 | 1.60 | 5 | 2 |
| 1:A:60:ILE:HG13 | 2:B:159:ILE:HB | 0.73 | 1.60 | 10 | 9 |
| 2:B:120:ALA:HB1 | 2:B:139:LEU:HD13 | 0.72 | 1.59 | 2 | 10 |
| 2:B:154:VAL:HB | 2:B:155:ILE:HD12 | 0.72 | 1.62 | 8 | 10 |
| 1:A:11:TYR:HB2 | 2:B:109:LEU:HD13 | 0.71 | 1.62 | 1 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:108:LEU:HD12 | 2:B:151:ILE:HG13 | 0.71 | 1.62 | 6 | 10 |
| 2:B:111:ALA:HA | 2:B:115:ASN:O | 0.71 | 1.85 | 10 | 10 |
| 1:A:5:SER:HB3 | 1:A:39:VAL:HA | 0.71 | 1.62 | 9 | 6 |
| 1:A:14:LEU:HD22 | 1:A:56:ILE:HD11 | 0.71 | 1.61 | 2 | 10 |
| 1:A:7:LEU:HA | 1:A:10:ILE:HD12 | 0.69 | 1.64 | 3 | 10 |
| 2:B:106:SER:HB2 | 2:B:123:ILE:HG23 | 0.69 | 1.64 | 6 | 10 |
| 2:B:135:ASP:HB2 | 2:B:138:ARG:HG3 | 0.68 | 1.66 | 10 | 8 |
| 2:B:124:LYS:HD3 | 2:B:139:LEU:HD21 | 0.67 | 1.65 | 3 | 8 |
| 2:B:107:TYR:O | 2:B:118:PRO:HG2 | 0.66 | 1.90 | 3 | 10 |
| 1:A:59:LEU:HB2 | 2:B:159:ILE:HG21 | 0.66 | 1.66 | 1 | 8 |
| 2:B:123:ILE:CG1 | 2:B:143:ILE:HD11 | 0.66 | 2.21 | 1 | 7 |
| 2:B:135:ASP:HB2 | 2:B:138:ARG:CG | 0.65 | 2.21 | 9 | 9 |
| 1:A:19:ASP:HB2 | 2:B:132:ILE:HG23 | 0.65 | 1.69 | 8 | 4 |
| 2:B:123:ILE:O | 2:B:127:LEU:HG | 0.65 | 1.92 | 1 | 9 |
| 1:A:24:THR:OG1 | 1:A:27:LYS:HG2 | 0.64 | 1.92 | 2 | 1 |
| 2:B:108:LEU:HG | 2:B:155:ILE:CD1 | 0.62 | 2.24 | 7 | 10 |
| 1:A:15:ILE:HD11 | 2:B:109:LEU:HD12 | 0.62 | 1.71 | 4 | 1 |
| 1:A:7:LEU:O | 1:A:10:ILE:HB | 0.61 | 1.95 | 7 | 10 |
| 2:B:155:ILE:O | 2:B:159:ILE:HD12 | 0.61 | 1.96 | 1 | 1 |
| 2:B:107:TYR:HD2 | 2:B:143:ILE:HG12 | 0.61 | 1.56 | 4 | 3 |
| 2:B:122:ASP:HA | 2:B:125:LYS:HE3 | 0.61 | 1.73 | 5 | 1 |
| 2:B:142:VAL:O | 2:B:146:LEU:HG | 0.61 | 1.95 | 2 | 5 |
| 2:B:140:ASN:O | 2:B:143:ILE:HB | 0.60 | 1.95 | 7 | 6 |
| 2:B:123:ILE:HG13 | 2:B:143:ILE:HD11 | 0.60 | 1.73 | 4 | 4 |
| 1:A:16:LEU:HD12 | 1:A:21:VAL:HG13 | 0.60 | 1.74 | 5 | 4 |
| 2:B:107:TYR:CG | 2:B:146:LEU:HD12 | 0.60 | 2.30 | 8 | 5 |
| 2:B:108:LEU:HG | 2:B:155:ILE:HD13 | 0.60 | 1.73 | 9 | 9 |
| 1:A:21:VAL:HG22 | 1:A:22:THR:H | 0.60 | 1.57 | 9 | 3 |
| 1:A:5:SER:HB2 | 1:A:39:VAL:HA | 0.59 | 1.74 | 1 | 2 |
| 2:B:107:TYR:CD2 | 2:B:143:ILE:HG12 | 0.59 | 2.32 | 4 | 4 |
| 2:B:155:ILE:HD12 | 2:B:155:ILE:N | 0.59 | 2.13 | 5 | 10 |
| 2:B:130:VAL:HG23 | 2:B:132:ILE:HG13 | 0.59 | 1.72 | 8 | 1 |
| 2:B:111:ALA:HB3 | 2:B:151:ILE:HG12 | 0.58 | 1.75 | 1 | 5 |
| 1:A:11:TYR:OH | 2:B:155:ILE:HB | 0.58 | 1.99 | 5 | 9 |
| 2:B:139:LEU:O | 2:B:142:VAL:HG12 | 0.58 | 1.99 | 2 | 10 |
| 1:A:11:TYR:CE2 | 2:B:112:LEU:HD22 | 0.57 | 2.34 | 1 | 3 |
| 1:A:60:ILE:CD1 | 2:B:159:ILE:HB | 0.57 | 2.29 | 3 | 9 |
| 1:A:60:ILE:CG1 | 2:B:159:ILE:HB | 0.57 | 2.28 | 10 | 6 |
| 2:B:146:LEU:O | 2:B:149:LYS:HB2 | 0.57 | 2.00 | 8 | 2 |
| 1:A:14:LEU:HB3 | 2:B:105:ALA:CB | 0.57 | 2.30 | 7 | 10 |
| 2:B:108:LEU:HG | 2:B:155:ILE:HD11 | 0.57 | 1.77 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:125:LYS:HD2 | 2:B:126:ILE:HD12 | 0.57 | 1.76 | 10 | 2 |
| 1:A:3:SER:HB2 | 1:A:6:GLU:HG3 | 0.56 | 1.78 | 3 | 2 |
| 2:B:112:LEU:HD11 | 2:B:152:GLU:HG3 | 0.56 | 1.77 | 5 | 4 |
| 1:A:37:VAL:HB | 2:B:113:GLY:CA | 0.56 | 2.25 | 1 | 9 |
| 1:A:31:LEU:HB3 | 2:B:109:LEU:HD21 | 0.56 | 1.76 | 9 | 6 |
| 2:B:107:TYR:CZ | 2:B:118:PRO:HD2 | 0.56 | 2.36 | 1 | 10 |
| 2:B:138:ARG:O | 2:B:141:LYS:HG3 | 0.56 | 2.01 | 3 | 1 |
| 1:A:32:ILE:HG23 | 1:A:37:VAL:O | 0.55 | 2.01 | 4 | 10 |
| 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 0.55 | 1.76 | 10 | 2 |
| 2:B:119:SER:O | 2:B:123:ILE:HG12 | 0.55 | 2.01 | 7 | 9 |
| 2:B:135:ASP:HB3 | 2:B:138:ARG:HG3 | 0.54 | 1.79 | 6 | 1 |
| 1:A:7:LEU:HD11 | 2:B:155:ILE:O | 0.54 | 2.02 | 4 | 3 |
| 2:B:106:SER:CB | 2:B:123:ILE:HG23 | 0.54 | 2.32 | 9 | 9 |
| 2:B:138:ARG:HA | 2:B:141:LYS:HE2 | 0.53 | 1.80 | 6 | 1 |
| 2:B:139:LEU:O | 2:B:143:ILE:HD12 | 0.53 | 2.03 | 3 | 4 |
| 2:B:135:ASP:HB3 | 2:B:138:ARG:CG | 0.53 | 2.33 | 6 | 1 |
| 2:B:104:VAL:HA | 2:B:146:LEU:HD11 | 0.53 | 1.81 | 9 | 2 |
| 2:B:138:ARG:O | 2:B:141:LYS:HG2 | 0.53 | 2.03 | 6 | 3 |
| 2:B:139:LEU:HA | 2:B:142:VAL:HG12 | 0.53 | 1.81 | 4 | 7 |
| 2:B:105:ALA:HA | 2:B:108:LEU:HD22 | 0.52 | 1.80 | 9 | 5 |
| 1:A:47:PHE:HD2 | 1:A:51:LEU:HD11 | 0.52 | 1.65 | 4 | 2 |
| 2:B:115:ASN:C | 2:B:117:SER:H | 0.52 | 2.08 | 10 | 6 |
| 2:B:141:LYS:O | 2:B:145:GLU:HG2 | 0.52 | 2.05 | 2 | 1 |
| 2:B:121:LYS:HD2 | 2:B:121:LYS:N | 0.51 | 2.20 | 6 | 3 |
| 1:A:23:VAL:HG12 | 1:A:48:ALA:HA | 0.51 | 1.81 | 10 | 6 |
| 2:B:122:ASP:O | 2:B:125:LYS:HB2 | 0.51 | 2.04 | 7 | 1 |
| 2:B:115:ASN:ND2 | 2:B:118:PRO:HA | 0.51 | 2.19 | 3 | 5 |
| 2:B:124:LYS:CD | 2:B:139:LEU:HD21 | 0.51 | 2.35 | 2 | 3 |
| 2:B:123:ILE:HG22 | 2:B:127:LEU:HD23 | 0.51 | 1.82 | 8 | 3 |
| 1:A:6:GLU:HG2 | 1:A:43:TRP:NE1 | 0.50 | 2.22 | 10 | 3 |
| 2:B:139:LEU:HD12 | 2:B:140:ASN:H | 0.50 | 1.65 | 10 | 5 |
| 2:B:136:ASP:CA | 2:B:139:LEU:HD11 | 0.50 | 2.24 | 6 | 3 |
| 2:B:135:ASP:O | 2:B:139:LEU:HG | 0.50 | 2.07 | 6 | 6 |
| 2:B:150:ASN:O | 2:B:154:VAL:HG23 | 0.50 | 2.06 | 6 | 8 |
| 2:B:104:VAL:O | 2:B:108:LEU:HD22 | 0.49 | 2.07 | 6 | 7 |
| 1:A:8:ALA:HB2 | 2:B:112:LEU:HD23 | 0.49 | 1.82 | 7 | 6 |
| 1:A:50:ALA:O | 1:A:54:VAL:HG22 | 0.49 | 2.07 | 2 | 1 |
| 1:A:43:TRP:CE3 | 1:A:47:PHE:HE1 | 0.49 | 2.25 | 1 | 5 |
| 2:B:120:ALA:HB1 | 2:B:139:LEU:CD1 | 0.49 | 2.36 | 6 | 4 |
| 1:A:24:THR:OG1 | 1:A:27:LYS:HB2 | 0.49 | 2.07 | 4 | 4 |
| 2:B:107:TYR:CZ | 2:B:146:LEU:HB3 | 0.48 | 2.42 | 6 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:107:TYR:CE1 | 2:B:118:PRO:HD2 | 0.48 | 2.43 | 8 | 1 |
| 1:A:10:ILE:HD13 | 2:B:159:ILE:CG1 | 0.48 | 2.38 | 5 | 3 |
| 1:A:47:PHE:CD2 | 1:A:51:LEU:HD11 | 0.48 | 2.43 | 1 | 1 |
| 1:A:7:LEU:HB3 | 2:B:112:LEU:HD21 | 0.48 | 1.84 | 1 | 3 |
| 1:A:16:LEU:HD21 | 1:A:23:VAL:HA | 0.48 | 1.85 | 6 | 2 |
| 1:A:29:ASN:HA | 1:A:32:ILE:HD12 | 0.48 | 1.84 | 5 | 1 |
| 1:A:40:GLU:HB2 | 1:A:43:TRP:CD1 | 0.48 | 2.44 | 6 | 2 |
| 1:A:34:ALA:HB1 | 2:B:126:ILE:HA | 0.48 | 1.85 | 10 | 2 |
| 2:B:135:ASP:OD1 | 2:B:138:ARG:HG2 | 0.48 | 2.08 | 6 | 1 |
| 2:B:139:LEU:HD12 | 2:B:140:ASN:N | 0.48 | 2.24 | 8 | 4 |
| 2:B:155:ILE:HG22 | 2:B:155:ILE:O | 0.48 | 2.08 | 10 | 5 |
| 1:A:10:ILE:HD13 | 2:B:159:ILE:HG13 | 0.47 | 1.85 | 2 | 3 |
| 2:B:117:SER:N | 2:B:118:PRO:HD3 | 0.47 | 2.24 | 4 | 10 |
| 1:A:21:VAL:HG22 | 1:A:22:THR:N | 0.47 | 2.24 | 9 | 4 |
| 1:A:37:VAL:CG1 | 2:B:109:LEU:HD23 | 0.47 | 2.40 | 4 | 1 |
| 1:A:11:TYR:HA | 1:A:14:LEU:HB2 | 0.47 | 1.86 | 3 | 8 |
| 1:A:24:THR:OG1 | 1:A:27:LYS:HE2 | 0.47 | 2.10 | 8 | 3 |
| 2:B:124:LYS:O | 2:B:128:ASP:HB2 | 0.47 | 2.10 | 10 | 4 |
| 2:B:155:ILE:O | 2:B:155:ILE:HG22 | 0.47 | 2.09 | 7 | 4 |
| 1:A:7:LEU:HD12 | 1:A:10:ILE:CD1 | 0.47 | 2.34 | 9 | 2 |
| 1:A:11:TYR:CE1 | 2:B:155:ILE:HG12 | 0.47 | 2.45 | 1 | 1 |
| 1:A:7:LEU:HD22 | 2:B:152:GLU:OE1 | 0.47 | 2.09 | 6 | 1 |
| 1:A:11:TYR:HE2 | 2:B:112:LEU:HD22 | 0.47 | 1.70 | 1 | 1 |
| 2:B:123:ILE:HG12 | 2:B:143:ILE:HD11 | 0.47 | 1.87 | 1 | 1 |
| 1:A:10:ILE:HG22 | 1:A:14:LEU:HD23 | 0.47 | 1.87 | 7 | 5 |
| 2:B:103:TYR:HB3 | 2:B:123:ILE:HG21 | 0.46 | 1.85 | 6 | 3 |
| 1:A:43:TRP:CE3 | 1:A:47:PHE:CE1 | 0.46 | 3.03 | 1 | 3 |
| 1:A:46:LEU:O | 1:A:49:LYS:HB2 | 0.46 | 2.11 | 1 | 1 |
| 2:B:125:LYS:CD | 2:B:126:ILE:HD12 | 0.46 | 2.40 | 10 | 2 |
| 2:B:146:LEU:O | 2:B:149:LYS:HE2 | 0.46 | 2.11 | 1 | 1 |
| 1:A:14:LEU:CD1 | 1:A:56:ILE:HG12 | 0.46 | 2.41 | 6 | 7 |
| 2:B:142:VAL:O | 2:B:146:LEU:HD23 | 0.46 | 2.11 | 1 | 2 |
| 1:A:11:TYR:O | 1:A:15:ILE:HG12 | 0.46 | 2.11 | 9 | 4 |
| 2:B:104:VAL:O | 2:B:107:TYR:HB3 | 0.45 | 2.11 | 4 | 5 |
| 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 0.45 | 1.88 | 5 | 1 |
| 1:A:9:CYS:HB2 | 1:A:39:VAL:HG11 | 0.45 | 1.88 | 8 | 3 |
| 2:B:119:SER:C | 2:B:143:ILE:HD13 | 0.45 | 2.31 | 1 | 3 |
| 1:A:39:VAL:HG12 | 1:A:40:GLU:N | 0.45 | 2.26 | 7 | 6 |
| 1:A:12:SER:HB2 | 1:A:28:ILE:HG23 | 0.45 | 1.89 | 4 | 1 |
| 2:B:104:VAL:HG12 | 2:B:108:LEU:HD21 | 0.45 | 1.89 | 9 | 2 |
| 1:A:10:ILE:HG22 | 1:A:14:LEU:CD2 | 0.45 | 2.42 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:140:ASN:HA | 2:B:143:ILE:CG1 | 0.45 | 2.42 | 5 | 2 |
| 2:B:107:TYR:CD1 | 2:B:146:LEU:HD12 | 0.44 | 2.47 | 2 | 2 |
| 1:A:35:ALA:CB | 2:B:109:LEU:HG | 0.44 | 2.42 | 7 | 2 |
| 2:B:124:LYS:HA | 2:B:127:LEU:HD11 | 0.44 | 1.89 | 7 | 2 |
| 2:B:127:LEU:HD13 | 2:B:132:ILE:O | 0.44 | 2.12 | 7 | 4 |
| 2:B:124:LYS:CD | 2:B:127:LEU:HD11 | 0.44 | 2.35 | 6 | 1 |
| 1:A:6:GLU:O | 1:A:10:ILE:HG13 | 0.44 | 2.13 | 3 | 6 |
| 1:A:16:LEU:CD1 | 1:A:21:VAL:HG13 | 0.44 | 2.41 | 5 | 1 |
| 2:B:104:VAL:HG12 | 2:B:108:LEU:CD2 | 0.44 | 2.43 | 10 | 5 |
| 1:A:49:LYS:HD2 | 1:A:49:LYS:O | 0.43 | 2.13 | 6 | 1 |
| 1:A:3:SER:HB2 | 1:A:6:GLU:OE1 | 0.43 | 2.14 | 8 | 1 |
| 2:B:110:ALA:HB3 | 2:B:118:PRO:HB3 | 0.43 | 1.90 | 10 | 1 |
| 2:B:140:ASN:HA | 2:B:143:ILE:HG12 | 0.43 | 1.91 | 7 | 3 |
| 1:A:40:GLU:HB3 | 1:A:43:TRP:HD1 | 0.43 | 1.74 | 7 | 1 |
| 1:A:5:SER:O | 1:A:39:VAL:HG22 | 0.43 | 2.14 | 4 | 2 |
| 1:A:27:LYS:O | 1:A:31:LEU:HD22 | 0.43 | 2.13 | 6 | 1 |
| 1:A:4:VAL:HG13 | 2:B:112:LEU:CG | 0.43 | 2.37 | 2 | 1 |
| 1:A:11:TYR:CD2 | 2:B:112:LEU:HD22 | 0.43 | 2.49 | 3 | 1 |
| 1:A:31:LEU:HD12 | 2:B:126:ILE:HG23 | 0.43 | 1.91 | 6 | 2 |
| 2:B:108:LEU:HD12 | 2:B:151:ILE:CG1 | 0.43 | 2.41 | 8 | 2 |
| 2:B:123:ILE:HB | 2:B:139:LEU:HD22 | 0.42 | 1.91 | 9 | 1 |
| 1:A:11:TYR:CE2 | 2:B:108:LEU:HB3 | 0.42 | 2.49 | 4 | 3 |
| 1:A:37:VAL:CB | 2:B:113:GLY:HA2 | 0.42 | 2.39 | 9 | 1 |
| 1:A:41:PRO:C | 1:A:44:PRO:HD2 | 0.42 | 2.35 | 7 | 3 |
| 1:A:16:LEU:HD12 | 1:A:21:VAL:CG1 | 0.42 | 2.43 | 5 | 1 |
| 1:A:24:THR:OG1 | 1:A:27:LYS:HD2 | 0.42 | 2.14 | 6 | 1 |
| 1:A:32:ILE:HG23 | 1:A:38:ASN:HA | 0.42 | 1.92 | 6 | 1 |
| 1:A:32:ILE:HG22 | 1:A:33:LYS:HD2 | 0.42 | 1.90 | 8 | 1 |
| 2:B:138:ARG:O | 2:B:141:LYS:HB3 | 0.41 | 2.14 | 9 | 1 |
| 1:A:11:TYR:CB | 2:B:109:LEU:HD13 | 0.41 | 2.40 | 9 | 1 |
| 1:A:6:GLU:HG2 | 1:A:43:TRP:HE1 | 0.41 | 1.74 | 10 | 2 |
| 1:A:40:GLU:O | 1:A:43:TRP:HB2 | 0.41 | 2.14 | 6 | 2 |
| 1:A:5:SER:CB | 1:A:39:VAL:HA | 0.41 | 2.44 | 1 | 1 |
| 2:B:111:ALA:CB | 2:B:151:ILE:HG12 | 0.41 | 2.45 | 1 | 2 |
| 2:B:155:ILE:HG23 | 2:B:159:ILE:HA | 0.41 | 1.92 | 4 | 1 |
| 1:A:17:HIS:CD2 | 1:A:56:ILE:HB | 0.41 | 2.50 | 9 | 1 |
| 1:A:16:LEU:HD11 | 1:A:27:LYS:HG2 | 0.41 | 1.93 | 7 | 2 |
| 2:B:151:ILE:HG22 | 2:B:152:GLU:N | 0.41 | 2.29 | 1 | 1 |
| 1:A:22:THR:O | 1:A:27:LYS:HG3 | 0.41 | 2.16 | 2 | 1 |
| 2:B:120:ALA:O | 2:B:124:LYS:HG2 | 0.41 | 2.15 | 4 | 1 |
| 2:B:127:LEU:HD12 | 2:B:128:ASP:N | 0.41 | 2.31 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:159:ILE:N | 2:B:159:ILE:HD12 | 0.41 | 2.31 | 10 | 1 |
| 2:B:108:LEU:CG | 2:B:155:ILE:HD11 | 0.41 | 2.43 | 1 | 1 |
| 2:B:122:ASP:O | 2:B:125:LYS:HB3 | 0.41 | 2.15 | 1 | 1 |
| 2:B:106:SER:HB2 | 2:B:123:ILE:HD12 | 0.40 | 1.91 | 1 | 1 |
| 2:B:103:TYR:OH | 2:B:134:ALA:HA | 0.40 | 2.16 | 4 | 1 |
| 1:A:16:LEU:HD12 | 1:A:16:LEU:HA | 0.40 | 1.72 | 9 | 1 |
| 1:A:34:ALA:HB2 | 2:B:129:SER:CB | 0.40 | 2.46 | 10 | 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 | 58/69 (84%) | 54±1 (93±3%) | 4±1 (7±3%) | 0±0 (0±0%) | 100 | 100 |
| 2 | B | 58/70 (83%) | 49±2 (84±3%) | 9±2 (15±4%) | 1±1 (1±1%) | 20 | 68 |
| All | All | 1160/1390 (83%) | 1026 (88%) | 128 (11%) | 6 (1%) | 32 | 76 |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | B | 114 | GLY | 5 |
| 2 | B | 151 | ILE | 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 | 47/52 (90%) | 42±1 (90±2%) | 5±1 (10±2%) | 11 | 57 |
| 2 | B | 46/53 (87%) | 41±1 (90±3%) | 5±1 (10±3%) | 11 | 56 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|----------------|-----------|----------|-------------|
| All | All | 930/1050 (89%) | 838 (90%) | 92 (10%) | 11 57 |

All 21 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 14 | LEU | 10 |
| 1 | A | 15 | ILE | 10 |
| 1 | A | 60 | ILE | 10 |
| 2 | B | 108 | LEU | 10 |
| 2 | B | 139 | LEU | 10 |
| 1 | A | 42 | PHE | 8 |
| 2 | B | 149 | LYS | 7 |
| 2 | B | 106 | SER | 4 |
| 2 | B | 121 | LYS | 4 |
| 2 | B | 125 | LYS | 3 |
| 1 | A | 26 | ASP | 3 |
| 2 | B | 141 | LYS | 2 |
| 1 | A | 49 | LYS | 2 |
| 2 | B | 146 | LEU | 2 |
| 2 | B | 150 | ASN | 1 |
| 2 | B | 109 | LEU | 1 |
| 2 | B | 116 | SER | 1 |
| 1 | A | 27 | LYS | 1 |
| 1 | A | 31 | LEU | 1 |
| 1 | A | 3 | SER | 1 |
| 2 | B | 128 | ASP | 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 69% for the well-defined parts and 68% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

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

| | |
|---|------|
| Total number of shifts | 1202 |
| Number of shifts mapped to atoms | 1202 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 1 |

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 138 | -0.38 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 122 | 0.06 ± 0.07 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 0 | — | None (insufficient data) |

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 69%, i.e. 1048 atoms were assigned a chemical shift out of a possible 1510. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 338/583 (58%) | 222/238 (93%) | 116/232 (50%) | 0/113 (0%) |
| Sidechain | 692/860 (80%) | 461/567 (81%) | 231/273 (85%) | 0/20 (0%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 18/67 (27%) | 18/32 (56%) | 0/32 (0%) | 0/3 (0%) |
| Overall | 1048/1510 (69%) | 701/837 (84%) | 347/537 (65%) | 0/136 (0%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 1202 atoms were assigned a chemical shift out of a possible 1765. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 399/699 (57%) | 261/287 (91%) | 138/278 (50%) | 0/134 (0%) |
| Sidechain | 785/999 (79%) | 522/661 (79%) | 263/313 (84%) | 0/25 (0%) |
| Aromatic | 18/67 (27%) | 18/32 (56%) | 0/32 (0%) | 0/3 (0%) |
| Overall | 1202/1765 (68%) | 801/980 (82%) | 401/623 (64%) | 0/162 (0%) |

7.1.4 Statistically unusual chemical shifts [i](#)

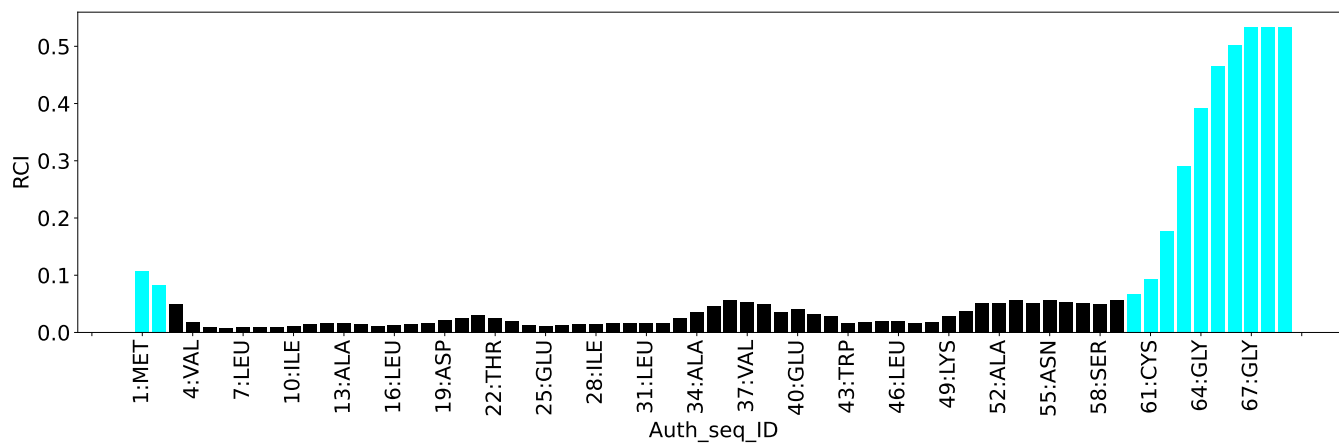
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 6 | GLU | HG2 | 1.04 | 1.24 – 3.30 | -6.0 |

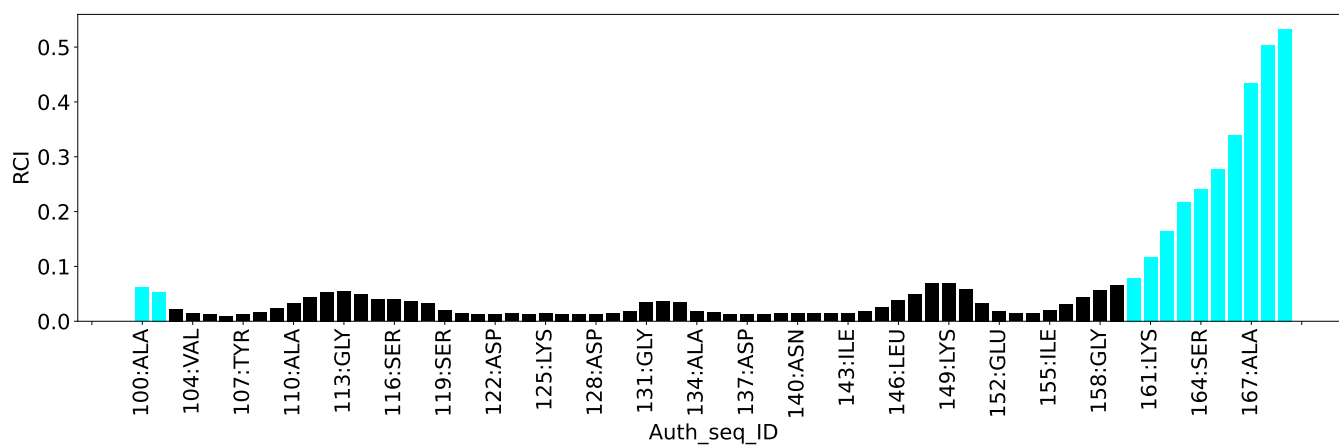
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 4675 |
| Intra-residue ($ i-j =0$) | 2419 |
| Sequential ($ i-j =1$) | 693 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 583 |
| Long range ($ i-j \geq 5$) | 453 |
| Inter-chain | 417 |
| Hydrogen bond restraints | 110 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 140 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 34.6 |
| Number of long range restraints per residue ¹ | 3.3 |

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) | 175.2 | 0.2 |
| 0.2-0.5 (Medium) | 112.3 | 0.5 |
| >0.5 (Large) | 147.4 | 4.33 |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 0.9 | 3.4 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis i

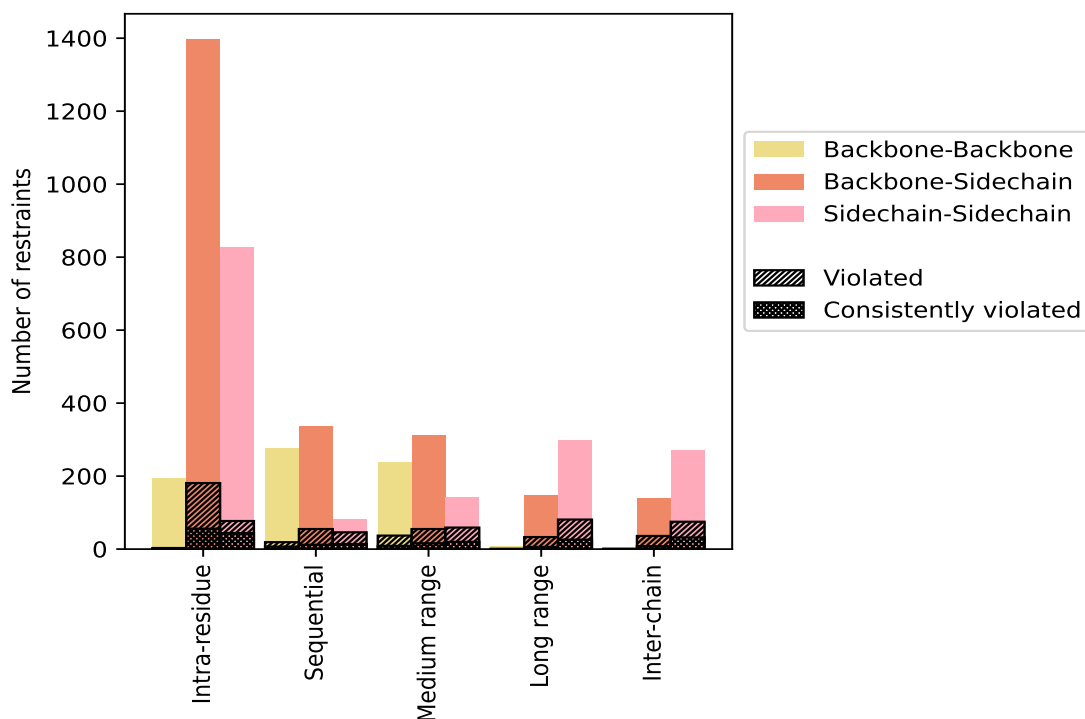
9.1 Summary of distance violations i

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 2419 | 51.7 | 261 | 10.8 | 5.6 | 101 | 4.2 | 2.2 |
| Backbone-Backbone | 194 | 4.1 | 3 | 1.5 | 0.1 | 1 | 0.5 | 0.0 |
| Backbone-Sidechain | 1397 | 29.9 | 181 | 13.0 | 3.9 | 56 | 4.0 | 1.2 |
| Sidechain-Sidechain | 828 | 17.7 | 77 | 9.3 | 1.6 | 44 | 5.3 | 0.9 |
| Sequential ($i-j =1$) | 693 | 14.8 | 120 | 17.3 | 2.6 | 33 | 4.8 | 0.7 |
| Backbone-Backbone | 276 | 5.9 | 19 | 6.9 | 0.4 | 7 | 2.5 | 0.1 |
| Backbone-Sidechain | 335 | 7.2 | 55 | 16.4 | 1.2 | 12 | 3.6 | 0.3 |
| Sidechain-Sidechain | 82 | 1.8 | 46 | 56.1 | 1.0 | 14 | 17.1 | 0.3 |
| Medium range ($i-j >1$ & $i-j <5$) | 583 | 12.5 | 122 | 20.9 | 2.6 | 38 | 6.5 | 0.8 |
| Backbone-Backbone | 128 | 2.7 | 8 | 6.2 | 0.2 | 2 | 1.6 | 0.0 |
| Backbone-Sidechain | 312 | 6.7 | 55 | 17.6 | 1.2 | 16 | 5.1 | 0.3 |
| Sidechain-Sidechain | 143 | 3.1 | 59 | 41.3 | 1.3 | 20 | 14.0 | 0.4 |
| Long range ($i-j \geq 5$) | 453 | 9.7 | 115 | 25.4 | 2.5 | 32 | 7.1 | 0.7 |
| Backbone-Backbone | 8 | 0.2 | 1 | 12.5 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 146 | 3.1 | 33 | 22.6 | 0.7 | 6 | 4.1 | 0.1 |
| Sidechain-Sidechain | 299 | 6.4 | 81 | 27.1 | 1.7 | 26 | 8.7 | 0.6 |
| Inter-chain | 417 | 8.9 | 112 | 26.9 | 2.4 | 40 | 9.6 | 0.9 |
| Backbone-Backbone | 6 | 0.1 | 1 | 16.7 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 140 | 3.0 | 36 | 25.7 | 0.8 | 8 | 5.7 | 0.2 |
| Sidechain-Sidechain | 271 | 5.8 | 75 | 27.7 | 1.6 | 32 | 11.8 | 0.7 |
| Hydrogen bond | 110 | 2.4 | 29 | 26.4 | 0.6 | 7 | 6.4 | 0.1 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 4675 | 100.0 | 759 | 16.2 | 16.2 | 251 | 5.4 | 5.4 |
| Backbone-Backbone | 722 | 15.4 | 61 | 8.4 | 1.3 | 17 | 2.4 | 0.4 |
| Backbone-Sidechain | 2330 | 49.8 | 360 | 15.5 | 7.7 | 98 | 4.2 | 2.1 |
| Sidechain-Sidechain | 1623 | 34.7 | 338 | 20.8 | 7.2 | 136 | 8.4 | 2.9 |

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](#)

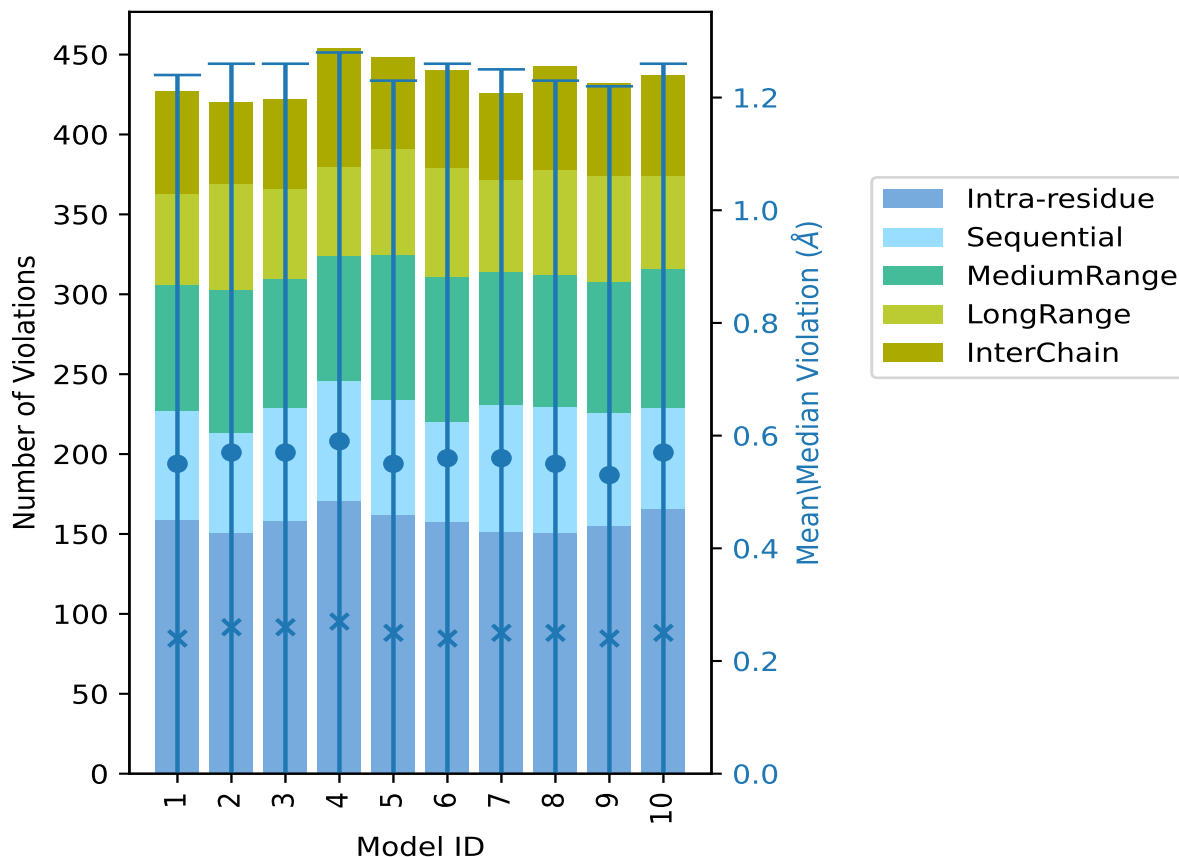
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| 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 | 159 | 68 | 79 | 57 | 64 | 427 | 0.55 | 4.21 | 0.69 | 0.24 |
| 2 | 151 | 62 | 90 | 66 | 51 | 420 | 0.57 | 4.3 | 0.69 | 0.26 |
| 3 | 158 | 71 | 81 | 56 | 56 | 422 | 0.57 | 4.27 | 0.69 | 0.26 |
| 4 | 171 | 75 | 78 | 56 | 74 | 454 | 0.59 | 4.3 | 0.69 | 0.27 |
| 5 | 162 | 72 | 91 | 66 | 57 | 448 | 0.55 | 4.3 | 0.68 | 0.25 |
| 6 | 158 | 62 | 91 | 68 | 61 | 440 | 0.56 | 4.33 | 0.7 | 0.24 |
| 7 | 151 | 80 | 83 | 58 | 54 | 426 | 0.56 | 4.24 | 0.69 | 0.25 |
| 8 | 151 | 79 | 82 | 66 | 65 | 443 | 0.55 | 4.32 | 0.68 | 0.25 |
| 9 | 155 | 71 | 82 | 66 | 58 | 432 | 0.53 | 4.33 | 0.69 | 0.24 |
| 10 | 166 | 63 | 87 | 58 | 63 | 437 | 0.57 | 4.28 | 0.69 | 0.25 |

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 [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3835(IR:2158, SQ:573, MR:461, LR:338, IC:305) 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 | % |
| 52 | 22 | 24 | 22 | 27 | 147 | 1 | 10.0 |
| 21 | 15 | 17 | 14 | 24 | 91 | 2 | 20.0 |
| 17 | 3 | 9 | 13 | 0 | 42 | 3 | 30.0 |
| 20 | 12 | 5 | 7 | 5 | 49 | 4 | 40.0 |

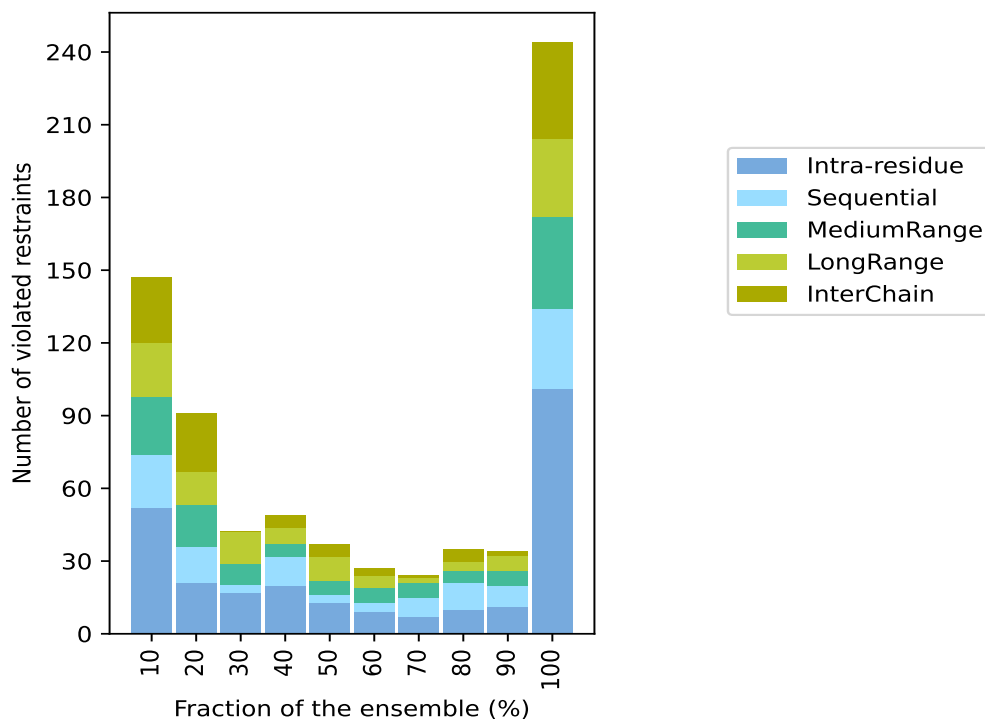
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 13 | 3 | 6 | 10 | 5 | 37 | 5 | 50.0 |
| 9 | 4 | 6 | 5 | 3 | 27 | 6 | 60.0 |
| 7 | 8 | 6 | 2 | 1 | 24 | 7 | 70.0 |
| 10 | 11 | 5 | 4 | 5 | 35 | 8 | 80.0 |
| 11 | 9 | 6 | 6 | 2 | 34 | 9 | 90.0 |
| 101 | 33 | 38 | 32 | 40 | 244 | 10 | 100.0 |

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

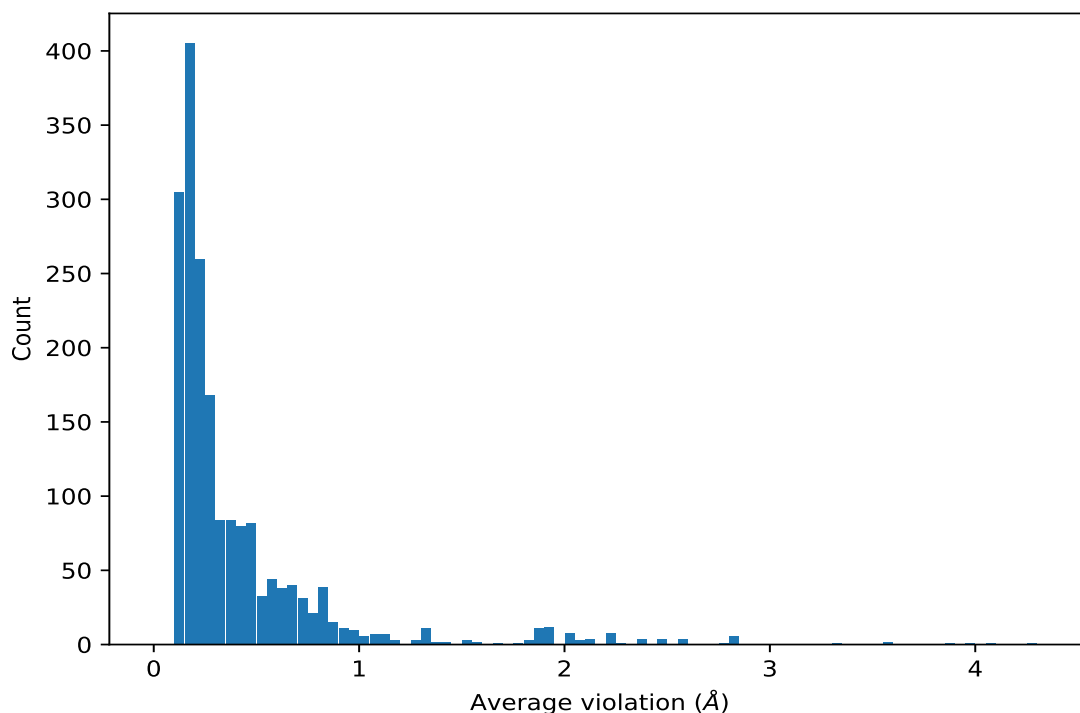
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 10 | 4.29 | 0.04 | 4.3 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 10 | 4.07 | 0.04 | 4.08 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 10 | 3.96 | 0.05 | 3.99 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 10 | 3.87 | 0.05 | 3.9 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 10 | 3.59 | 0.15 | 3.59 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 10 | 3.59 | 0.15 | 3.59 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 10 | 3.3 | 0.05 | 3.3 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 10 | 2.81 | 0.06 | 2.8 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 10 | 2.81 | 0.06 | 2.8 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 10 | 2.81 | 0.06 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 10 | 2.81 | 0.06 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 10 | 2.81 | 0.06 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 10 | 2.81 | 0.06 | 2.8 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 10 | 2.77 | 0.05 | 2.78 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 10 | 2.58 | 0.08 | 2.6 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 10 | 2.58 | 0.08 | 2.6 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 10 | 2.56 | 0.08 | 2.58 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 10 | 2.56 | 0.08 | 2.58 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 10 | 2.49 | 0.08 | 2.48 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 10 | 2.49 | 0.08 | 2.48 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 10 | 2.49 | 0.08 | 2.48 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 10 | 2.49 | 0.05 | 2.5 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 10 | 2.36 | 0.08 | 2.38 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 10 | 2.36 | 0.08 | 2.38 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 10 | 2.36 | 0.08 | 2.38 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 2.36 | 0.08 | 2.38 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 10 | 2.28 | 0.05 | 2.29 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 2.2 | 0.08 | 2.22 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 10 | 2.2 | 0.08 | 2.22 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 10 | 2.2 | 0.08 | 2.22 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 10 | 2.2 | 0.08 | 2.22 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 10 | 2.2 | 0.08 | 2.22 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 10 | 2.2 | 0.08 | 2.22 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 2.2 | 0.08 | 2.22 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 10 | 2.2 | 0.08 | 2.22 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 10 | 2.13 | 0.09 | 2.14 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 10 | 2.13 | 0.09 | 2.14 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 10 | 2.13 | 0.09 | 2.14 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 10 | 2.13 | 0.09 | 2.14 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 10 | 2.05 | 0.08 | 2.04 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 10 | 2.05 | 0.08 | 2.04 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 10 | 2.05 | 0.08 | 2.04 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 10 | 2.03 | 0.13 | 1.98 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 10 | 2.03 | 0.13 | 1.98 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 10 | 2.03 | 0.13 | 1.98 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 10 | 2.03 | 0.13 | 1.98 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 10 | 2.03 | 0.13 | 1.98 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 10 | 2.03 | 0.13 | 1.98 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 10 | 2.03 | 0.07 | 2.01 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 10 | 2.03 | 0.07 | 2.01 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 10 | 1.94 | 0.08 | 1.92 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 10 | 1.94 | 0.08 | 1.92 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 10 | 1.94 | 0.08 | 1.92 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 10 | 1.93 | 0.15 | 1.94 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 10 | 1.93 | 0.15 | 1.94 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 10 | 1.93 | 0.15 | 1.94 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 10 | 1.92 | 0.1 | 1.88 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 10 | 1.92 | 0.1 | 1.88 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 10 | 1.92 | 0.1 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 10 | 1.92 | 0.1 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 10 | 1.92 | 0.1 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 10 | 1.92 | 0.1 | 1.88 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 10 | 1.88 | 0.08 | 1.9 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 10 | 1.88 | 0.08 | 1.9 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 10 | 1.86 | 0.13 | 1.88 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 10 | 1.84 | 0.15 | 1.85 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 10 | 1.84 | 0.15 | 1.85 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 10 | 1.84 | 0.15 | 1.85 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 10 | 1.79 | 0.03 | 1.8 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 10 | 1.66 | 0.07 | 1.65 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 10 | 1.57 | 0.07 | 1.6 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 10 | 1.57 | 0.07 | 1.6 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 10 | 1.54 | 0.05 | 1.53 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 10 | 1.54 | 0.05 | 1.53 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 10 | 1.52 | 0.01 | 1.52 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 10 | 1.44 | 0.07 | 1.46 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 10 | 1.44 | 0.07 | 1.46 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 10 | 1.38 | 0.05 | 1.39 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 10 | 1.36 | 0.01 | 1.36 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 10 | 1.34 | 0.11 | 1.36 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 10 | 1.34 | 0.11 | 1.36 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 10 | 1.34 | 0.11 | 1.36 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 10 | 1.34 | 0.11 | 1.36 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 10 | 1.34 | 0.09 | 1.34 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 10 | 1.32 | 0.04 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 10 | 1.32 | 0.04 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 10 | 1.32 | 0.04 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 10 | 1.32 | 0.04 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 10 | 1.32 | 0.04 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 10 | 1.32 | 0.04 | 1.33 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 10 | 1.26 | 0.06 | 1.25 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 10 | 1.26 | 0.06 | 1.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 10 | 1.26 | 0.06 | 1.25 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 10 | 1.19 | 0.06 | 1.18 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 10 | 1.19 | 0.06 | 1.18 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 10 | 1.19 | 0.06 | 1.18 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 10 | 1.14 | 0.12 | 1.13 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 10 | 1.14 | 0.12 | 1.13 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 10 | 1.13 | 0.06 | 1.12 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 10 | 1.11 | 0.11 | 1.12 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 10 | 1.11 | 0.11 | 1.12 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 10 | 1.11 | 0.11 | 1.12 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 10 | 1.11 | 0.11 | 1.12 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 10 | 1.09 | 0.07 | 1.11 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 10 | 1.09 | 0.07 | 1.11 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 10 | 1.05 | 0.11 | 1.1 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 10 | 1.05 | 0.11 | 1.1 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 10 | 1.03 | 0.32 | 1.18 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 10 | 1.01 | 0.0 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 10 | 1.01 | 0.0 | 1.01 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 10 | 1.0 | 0.32 | 1.15 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 10 | 1.0 | 0.33 | 1.06 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 10 | 1.0 | 0.33 | 1.06 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.97 | 0.01 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.97 | 0.01 | 0.97 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 10 | 0.96 | 0.04 | 0.96 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 10 | 0.96 | 0.04 | 0.96 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 10 | 0.96 | 0.04 | 0.96 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 10 | 0.96 | 0.04 | 0.96 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 10 | 0.96 | 0.04 | 0.96 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 10 | 0.96 | 0.04 | 0.96 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 10 | 0.95 | 0.08 | 0.95 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 10 | 0.95 | 0.02 | 0.94 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 10 | 0.94 | 0.07 | 0.94 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 10 | 0.92 | 0.51 | 1.04 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 10 | 0.92 | 0.51 | 1.04 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 10 | 0.92 | 0.51 | 1.04 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 10 | 0.92 | 0.1 | 0.89 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 10 | 0.92 | 0.1 | 0.89 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 10 | 0.92 | 0.1 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.89 | 0.01 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.89 | 0.01 | 0.89 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 10 | 0.89 | 0.24 | 0.98 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 10 | 0.88 | 0.12 | 0.86 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 10 | 0.88 | 0.12 | 0.86 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 10 | 0.88 | 0.12 | 0.86 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 10 | 0.87 | 0.11 | 0.84 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 10 | 0.87 | 0.0 | 0.87 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 10 | 0.87 | 0.1 | 0.84 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 10 | 0.87 | 0.1 | 0.84 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 10 | 0.86 | 0.01 | 0.86 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.85 | 0.01 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.85 | 0.01 | 0.85 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 0.84 | 0.04 | 0.85 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 10 | 0.84 | 0.04 | 0.85 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 10 | 0.84 | 0.04 | 0.85 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 10 | 0.82 | 0.02 | 0.82 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 10 | 0.82 | 0.02 | 0.82 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 10 | 0.82 | 0.6 | 0.8 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 10 | 0.82 | 0.6 | 0.8 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 10 | 0.82 | 0.6 | 0.8 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 10 | 0.82 | 0.6 | 0.8 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 10 | 0.82 | 0.0 | 0.82 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 10 | 0.82 | 0.09 | 0.82 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 10 | 0.82 | 0.02 | 0.81 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 10 | 0.81 | 0.09 | 0.8 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 10 | 0.81 | 0.09 | 0.8 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.8 | 0.15 | 0.74 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.8 | 0.15 | 0.74 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.8 | 0.15 | 0.74 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 10 | 0.8 | 0.05 | 0.82 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 10 | 0.8 | 0.32 | 0.94 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 10 | 0.78 | 0.3 | 0.88 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 10 | 0.78 | 0.1 | 0.75 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 10 | 0.78 | 0.1 | 0.75 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 10 | 0.78 | 0.1 | 0.75 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 10 | 0.75 | 0.02 | 0.75 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 10 | 0.75 | 0.02 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 10 | 0.74 | 0.09 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 10 | 0.74 | 0.09 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 10 | 0.74 | 0.09 | 0.75 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 10 | 0.72 | 0.05 | 0.7 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 10 | 0.72 | 0.05 | 0.7 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 10 | 0.71 | 0.3 | 0.86 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 10 | 0.71 | 0.3 | 0.86 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.7 | 0.01 | 0.7 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.7 | 0.01 | 0.7 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 10 | 0.69 | 0.19 | 0.75 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 10 | 0.69 | 0.19 | 0.75 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 10 | 0.69 | 0.19 | 0.75 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 10 | 0.69 | 0.19 | 0.75 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.69 | 0.15 | 0.64 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.69 | 0.15 | 0.64 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.69 | 0.15 | 0.64 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 10 | 0.68 | 0.09 | 0.66 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 10 | 0.68 | 0.09 | 0.66 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 10 | 0.66 | 0.17 | 0.59 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 10 | 0.66 | 0.17 | 0.59 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.66 | 0.15 | 0.6 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.66 | 0.15 | 0.6 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.66 | 0.15 | 0.6 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.66 | 0.15 | 0.6 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.66 | 0.15 | 0.6 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.66 | 0.15 | 0.6 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 10 | 0.66 | 0.0 | 0.66 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 10 | 0.62 | 0.11 | 0.62 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 10 | 0.62 | 0.11 | 0.62 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 10 | 0.62 | 0.11 | 0.62 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 10 | 0.62 | 0.11 | 0.62 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 10 | 0.62 | 0.11 | 0.62 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 10 | 0.62 | 0.11 | 0.62 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 10 | 0.62 | 0.18 | 0.71 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 10 | 0.62 | 0.18 | 0.71 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 10 | 0.62 | 0.18 | 0.71 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 10 | 0.61 | 0.18 | 0.7 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 10 | 0.61 | 0.18 | 0.7 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 10 | 0.61 | 0.18 | 0.7 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 10 | 0.61 | 0.09 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 10 | 0.61 | 0.09 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 10 | 0.61 | 0.09 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 10 | 0.61 | 0.09 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 10 | 0.61 | 0.09 | 0.64 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 10 | 0.6 | 0.05 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 10 | 0.59 | 0.03 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 10 | 0.59 | 0.03 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 10 | 0.59 | 0.03 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 10 | 0.59 | 0.03 | 0.61 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 10 | 0.59 | 0.36 | 0.83 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 10 | 0.59 | 0.36 | 0.83 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 10 | 0.59 | 0.36 | 0.83 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 10 | 0.59 | 0.36 | 0.83 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 10 | 0.59 | 0.36 | 0.83 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 10 | 0.59 | 0.36 | 0.83 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 10 | 0.58 | 0.08 | 0.58 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 10 | 0.56 | 0.11 | 0.6 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 10 | 0.56 | 0.11 | 0.6 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 10 | 0.56 | 0.04 | 0.57 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 0.56 | 0.04 | 0.57 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 10 | 0.56 | 0.04 | 0.57 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 10 | 0.55 | 0.13 | 0.59 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 10 | 0.55 | 0.13 | 0.59 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 10 | 0.55 | 0.09 | 0.58 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 10 | 0.55 | 0.09 | 0.58 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 10 | 0.55 | 0.09 | 0.58 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 10 | 0.55 | 0.09 | 0.58 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 10 | 0.55 | 0.09 | 0.58 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 10 | 0.55 | 0.08 | 0.55 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 10 | 0.55 | 0.08 | 0.55 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 10 | 0.55 | 0.09 | 0.53 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 10 | 0.55 | 0.09 | 0.53 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 10 | 0.55 | 0.18 | 0.64 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 10 | 0.55 | 0.18 | 0.64 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 10 | 0.55 | 0.18 | 0.64 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 10 | 0.54 | 0.16 | 0.5 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 10 | 0.54 | 0.16 | 0.5 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 10 | 0.54 | 0.16 | 0.5 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 10 | 0.54 | 0.16 | 0.5 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.54 | 0.15 | 0.48 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.54 | 0.15 | 0.48 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.54 | 0.15 | 0.48 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 0.53 | 0.04 | 0.54 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 10 | 0.53 | 0.04 | 0.54 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 10 | 0.53 | 0.04 | 0.54 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 10 | 0.53 | 0.05 | 0.56 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 10 | 0.51 | 0.02 | 0.52 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 10 | 0.51 | 0.05 | 0.54 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 10 | 0.49 | 0.05 | 0.48 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 10 | 0.49 | 0.05 | 0.48 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 10 | 0.48 | 0.09 | 0.48 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 10 | 0.48 | 0.09 | 0.48 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 10 | 0.48 | 0.09 | 0.48 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 10 | 0.48 | 0.09 | 0.48 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 10 | 0.48 | 0.09 | 0.48 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 10 | 0.48 | 0.09 | 0.48 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 10 | 0.48 | 0.09 | 0.48 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 10 | 0.48 | 0.09 | 0.48 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 10 | 0.48 | 0.01 | 0.48 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 10 | 0.48 | 0.08 | 0.49 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 10 | 0.48 | 0.08 | 0.49 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 10 | 0.48 | 0.08 | 0.49 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 10 | 0.48 | 0.18 | 0.57 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 10 | 0.48 | 0.18 | 0.57 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 10 | 0.48 | 0.18 | 0.57 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 10 | 0.47 | 0.0 | 0.47 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 10 | 0.46 | 0.01 | 0.46 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 10 | 0.46 | 0.02 | 0.46 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 10 | 0.45 | 0.01 | 0.45 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 10 | 0.43 | 0.22 | 0.28 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 10 | 0.41 | 0.01 | 0.41 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 10 | 0.38 | 0.15 | 0.44 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 10 | 0.37 | 0.02 | 0.37 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 10 | 0.37 | 0.04 | 0.38 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 10 | 0.37 | 0.04 | 0.38 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 10 | 0.37 | 0.04 | 0.38 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 10 | 0.37 | 0.63 | 0.16 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 10 | 0.37 | 0.63 | 0.16 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 10 | 0.37 | 0.63 | 0.16 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 10 | 0.35 | 0.06 | 0.35 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 10 | 0.32 | 0.02 | 0.32 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 10 | 0.31 | 0.02 | 0.32 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 10 | 0.3 | 0.04 | 0.3 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 10 | 0.3 | 0.04 | 0.3 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 10 | 0.3 | 0.01 | 0.3 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.29 | 0.0 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.29 | 0.0 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.29 | 0.0 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.29 | 0.0 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.29 | 0.0 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.29 | 0.0 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.29 | 0.0 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.29 | 0.0 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.29 | 0.0 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.29 | 0.0 | 0.29 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 10 | 0.28 | 0.1 | 0.26 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 10 | 0.28 | 0.1 | 0.26 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 10 | 0.28 | 0.1 | 0.26 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.28 | 0.0 | 0.28 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 10 | 0.28 | 0.13 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 10 | 0.28 | 0.13 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 10 | 0.28 | 0.13 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 10 | 0.28 | 0.13 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 10 | 0.28 | 0.13 | 0.2 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.27 | 0.0 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.27 | 0.0 | 0.27 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 0.27 | 0.04 | 0.28 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 10 | 0.27 | 0.04 | 0.28 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 10 | 0.27 | 0.04 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 10 | 0.26 | 0.03 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 10 | 0.26 | 0.03 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 10 | 0.26 | 0.03 | 0.28 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.26 | 0.01 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.26 | 0.01 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 10 | 0.26 | 0.0 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 10 | 0.26 | 0.0 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 10 | 0.26 | 0.0 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 10 | 0.26 | 0.0 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 10 | 0.26 | 0.0 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 10 | 0.26 | 0.0 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 10 | 0.26 | 0.0 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 10 | 0.26 | 0.0 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 10 | 0.26 | 0.0 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 10 | 0.26 | 0.0 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 10 | 0.26 | 0.01 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 10 | 0.26 | 0.01 | 0.26 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 10 | 0.26 | 0.02 | 0.26 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 10 | 0.26 | 0.02 | 0.26 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 10 | 0.26 | 0.04 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 10 | 0.26 | 0.04 | 0.28 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 10 | 0.25 | 0.02 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 10 | 0.25 | 0.01 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 10 | 0.25 | 0.01 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 10 | 0.25 | 0.01 | 0.25 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 10 | 0.25 | 0.06 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 10 | 0.25 | 0.06 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 10 | 0.25 | 0.06 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 10 | 0.25 | 0.06 | 0.23 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 10 | 0.25 | 0.0 | 0.25 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 10 | 0.25 | 0.04 | 0.26 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 10 | 0.25 | 0.04 | 0.26 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 10 | 0.25 | 0.04 | 0.26 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 10 | 0.25 | 0.01 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 10 | 0.25 | 0.01 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 10 | 0.25 | 0.01 | 0.24 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 10 | 0.25 | 0.01 | 0.24 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 10 | 0.24 | 0.05 | 0.24 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 10 | 0.24 | 0.05 | 0.24 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 10 | 0.24 | 0.05 | 0.24 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 10 | 0.24 | 0.05 | 0.24 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 10 | 0.23 | 0.0 | 0.23 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 10 | 0.23 | 0.0 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 10 | 0.23 | 0.0 | 0.23 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 10 | 0.23 | 0.01 | 0.23 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 10 | 0.23 | 0.01 | 0.23 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 10 | 0.23 | 0.02 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 10 | 0.23 | 0.0 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 10 | 0.23 | 0.01 | 0.23 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 10 | 0.23 | 0.21 | 0.16 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 10 | 0.23 | 0.21 | 0.16 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 10 | 0.23 | 0.21 | 0.16 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 10 | 0.22 | 0.03 | 0.22 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 10 | 0.22 | 0.03 | 0.22 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 10 | 0.22 | 0.04 | 0.24 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 10 | 0.22 | 0.02 | 0.22 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 10 | 0.22 | 0.02 | 0.22 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 10 | 0.22 | 0.02 | 0.22 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 10 | 0.22 | 0.02 | 0.22 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 10 | 0.22 | 0.02 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 10 | 0.22 | 0.02 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 10 | 0.22 | 0.02 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 10 | 0.22 | 0.02 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 10 | 0.22 | 0.02 | 0.21 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 10 | 0.22 | 0.02 | 0.22 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 10 | 0.22 | 0.02 | 0.22 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 10 | 0.22 | 0.02 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 10 | 0.21 | 0.0 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 10 | 0.21 | 0.05 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 10 | 0.21 | 0.05 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 10 | 0.21 | 0.05 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 10 | 0.21 | 0.05 | 0.24 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 10 | 0.21 | 0.0 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 10 | 0.21 | 0.03 | 0.22 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 10 | 0.21 | 0.03 | 0.22 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 10 | 0.21 | 0.03 | 0.22 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 10 | 0.21 | 0.02 | 0.2 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 10 | 0.21 | 0.03 | 0.2 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 10 | 0.21 | 0.03 | 0.2 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 10 | 0.21 | 0.0 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 10 | 0.21 | 0.0 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 10 | 0.21 | 0.0 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 10 | 0.21 | 0.04 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 10 | 0.21 | 0.04 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 10 | 0.21 | 0.04 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 10 | 0.21 | 0.04 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 10 | 0.21 | 0.04 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 10 | 0.21 | 0.04 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 10 | 0.21 | 0.04 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 10 | 0.21 | 0.04 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 10 | 0.21 | 0.04 | 0.22 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 10 | 0.2 | 0.01 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 10 | 0.2 | 0.01 | 0.2 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 10 | 0.2 | 0.03 | 0.2 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 10 | 0.2 | 0.03 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 10 | 0.2 | 0.01 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 10 | 0.2 | 0.01 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 10 | 0.2 | 0.01 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.2 | 0.0 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.2 | 0.0 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.2 | 0.0 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.2 | 0.0 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.2 | 0.0 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.2 | 0.0 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.2 | 0.0 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.2 | 0.0 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.2 | 0.0 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.2 | 0.0 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.2 | 0.0 | 0.2 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 10 | 0.2 | 0.02 | 0.2 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 10 | 0.2 | 0.02 | 0.2 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 10 | 0.19 | 0.05 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 10 | 0.19 | 0.03 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 10 | 0.19 | 0.03 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 10 | 0.19 | 0.03 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 10 | 0.19 | 0.03 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 10 | 0.19 | 0.03 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 10 | 0.19 | 0.03 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 10 | 0.19 | 0.03 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 10 | 0.19 | 0.03 | 0.2 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 10 | 0.19 | 0.02 | 0.2 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 10 | 0.19 | 0.02 | 0.2 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 10 | 0.19 | 0.02 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 10 | 0.19 | 0.0 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 10 | 0.19 | 0.0 | 0.19 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 10 | 0.19 | 0.01 | 0.19 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 10 | 0.19 | 0.03 | 0.2 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 10 | 0.19 | 0.03 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 10 | 0.19 | 0.02 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 10 | 0.19 | 0.02 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 10 | 0.19 | 0.02 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 10 | 0.19 | 0.02 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 10 | 0.19 | 0.01 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 10 | 0.19 | 0.01 | 0.19 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 10 | 0.18 | 0.03 | 0.17 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 10 | 0.18 | 0.03 | 0.17 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 10 | 0.18 | 0.04 | 0.19 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.18 | 0.01 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.18 | 0.01 | 0.18 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 10 | 0.18 | 0.03 | 0.18 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 10 | 0.18 | 0.03 | 0.18 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 10 | 0.18 | 0.01 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.18 | 0.0 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 10 | 0.18 | 0.02 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 10 | 0.18 | 0.02 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 10 | 0.18 | 0.02 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 10 | 0.18 | 0.0 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 10 | 0.18 | 0.0 | 0.18 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 10 | 0.18 | 0.02 | 0.17 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 10 | 0.17 | 0.03 | 0.16 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 10 | 0.17 | 0.03 | 0.16 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 10 | 0.17 | 0.04 | 0.18 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 10 | 0.17 | 0.04 | 0.18 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 10 | 0.17 | 0.04 | 0.18 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 10 | 0.17 | 0.04 | 0.18 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 10 | 0.17 | 0.04 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 10 | 0.17 | 0.04 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 10 | 0.17 | 0.04 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 10 | 0.17 | 0.04 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 10 | 0.17 | 0.04 | 0.16 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 10 | 0.17 | 0.01 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 10 | 0.17 | 0.01 | 0.17 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 10 | 0.17 | 0.03 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 10 | 0.17 | 0.03 | 0.18 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 10 | 0.17 | 0.03 | 0.18 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 10 | 0.17 | 0.01 | 0.17 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 10 | 0.17 | 0.01 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 10 | 0.17 | 0.01 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 10 | 0.17 | 0.01 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 10 | 0.17 | 0.01 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 10 | 0.17 | 0.01 | 0.17 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 10 | 0.17 | 0.04 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 10 | 0.17 | 0.03 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 10 | 0.17 | 0.03 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 10 | 0.17 | 0.03 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 10 | 0.17 | 0.03 | 0.17 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 10 | 0.16 | 0.01 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 10 | 0.16 | 0.01 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 10 | 0.16 | 0.0 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 10 | 0.16 | 0.0 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 10 | 0.16 | 0.0 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 10 | 0.16 | 0.0 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 10 | 0.16 | 0.0 | 0.16 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 10 | 0.16 | 0.01 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 10 | 0.16 | 0.0 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 10 | 0.16 | 0.0 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 10 | 0.16 | 0.0 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 10 | 0.16 | 0.0 | 0.16 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 10 | 0.16 | 0.05 | 0.14 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 10 | 0.16 | 0.05 | 0.14 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 10 | 0.16 | 0.05 | 0.14 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 10 | 0.16 | 0.05 | 0.14 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 10 | 0.16 | 0.0 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 10 | 0.16 | 0.0 | 0.16 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 10 | 0.16 | 0.0 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 10 | 0.15 | 0.0 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 10 | 0.15 | 0.0 | 0.15 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 10 | 0.15 | 0.02 | 0.16 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 10 | 0.15 | 0.02 | 0.16 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 10 | 0.15 | 0.01 | 0.16 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 10 | 0.15 | 0.02 | 0.16 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 10 | 0.15 | 0.02 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 10 | 0.15 | 0.01 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 10 | 0.15 | 0.01 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 10 | 0.15 | 0.01 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 10 | 0.15 | 0.02 | 0.16 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 10 | 0.15 | 0.02 | 0.15 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 10 | 0.15 | 0.02 | 0.15 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 10 | 0.15 | 0.02 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 10 | 0.15 | 0.0 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 10 | 0.15 | 0.0 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 10 | 0.15 | 0.0 | 0.15 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 10 | 0.15 | 0.0 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 10 | 0.14 | 0.01 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 10 | 0.14 | 0.01 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 10 | 0.14 | 0.01 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 10 | 0.14 | 0.0 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 10 | 0.14 | 0.0 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 10 | 0.14 | 0.0 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 10 | 0.14 | 0.0 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 10 | 0.14 | 0.02 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 10 | 0.14 | 0.02 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 10 | 0.14 | 0.02 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 10 | 0.14 | 0.02 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 10 | 0.14 | 0.02 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 10 | 0.14 | 0.02 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 10 | 0.14 | 0.0 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 10 | 0.14 | 0.0 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 10 | 0.14 | 0.0 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 10 | 0.14 | 0.0 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 10 | 0.14 | 0.0 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 10 | 0.14 | 0.0 | 0.14 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 10 | 0.14 | 0.01 | 0.14 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 10 | 0.13 | 0.01 | 0.14 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 10 | 0.13 | 0.01 | 0.14 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.13 | 0.0 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.13 | 0.0 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 10 | 0.13 | 0.0 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 10 | 0.13 | 0.0 | 0.13 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 10 | 0.13 | 0.01 | 0.13 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 10 | 0.13 | 0.0 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 10 | 0.13 | 0.0 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 10 | 0.13 | 0.0 | 0.13 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 10 | 0.13 | 0.0 | 0.13 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 10 | 0.12 | 0.0 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 10 | 0.12 | 0.0 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.12 | 0.0 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.12 | 0.0 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.12 | 0.0 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.12 | 0.0 | 0.12 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 9 | 0.86 | 0.21 | 0.88 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 9 | 0.86 | 0.21 | 0.88 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 9 | 0.84 | 0.21 | 0.86 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 9 | 0.84 | 0.21 | 0.86 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 9 | 0.79 | 0.1 | 0.78 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 9 | 0.79 | 0.1 | 0.78 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 9 | 0.79 | 0.1 | 0.78 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 9 | 0.79 | 0.1 | 0.78 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 9 | 0.65 | 0.16 | 0.64 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 9 | 0.65 | 0.16 | 0.64 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 9 | 0.65 | 0.16 | 0.64 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 9 | 0.65 | 0.16 | 0.64 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 9 | 0.61 | 0.18 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 9 | 0.61 | 0.18 | 0.65 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 9 | 0.6 | 0.11 | 0.6 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 9 | 0.6 | 0.11 | 0.6 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 9 | 0.6 | 0.11 | 0.6 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 9 | 0.6 | 0.11 | 0.6 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 9 | 0.6 | 0.1 | 0.58 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 9 | 0.58 | 0.1 | 0.57 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 9 | 0.58 | 0.1 | 0.57 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 9 | 0.58 | 0.1 | 0.57 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 9 | 0.58 | 0.1 | 0.57 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 9 | 0.52 | 0.21 | 0.54 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 9 | 0.52 | 0.21 | 0.54 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 9 | 0.5 | 0.11 | 0.5 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 9 | 0.5 | 0.11 | 0.5 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 9 | 0.5 | 0.11 | 0.5 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 9 | 0.5 | 0.11 | 0.5 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 9 | 0.49 | 0.14 | 0.55 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 9 | 0.49 | 0.14 | 0.55 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 9 | 0.48 | 0.14 | 0.54 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 9 | 0.48 | 0.14 | 0.54 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 9 | 0.44 | 0.56 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 9 | 0.44 | 0.56 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 9 | 0.44 | 0.56 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 9 | 0.44 | 0.56 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 9 | 0.44 | 0.56 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 9 | 0.44 | 0.56 | 0.28 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 9 | 0.42 | 0.29 | 0.23 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 9 | 0.42 | 0.29 | 0.23 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 9 | 0.42 | 0.29 | 0.23 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 9 | 0.39 | 0.34 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 9 | 0.39 | 0.34 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 9 | 0.39 | 0.34 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 9 | 0.39 | 0.34 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 9 | 0.39 | 0.34 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 9 | 0.39 | 0.34 | 0.17 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 9 | 0.29 | 0.13 | 0.26 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 9 | 0.29 | 0.13 | 0.26 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 9 | 0.29 | 0.13 | 0.26 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 9 | 0.25 | 0.03 | 0.26 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 9 | 0.21 | 0.06 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 9 | 0.21 | 0.06 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 9 | 0.21 | 0.06 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 9 | 0.21 | 0.06 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 9 | 0.21 | 0.06 | 0.22 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 9 | 0.2 | 0.07 | 0.18 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 9 | 0.2 | 0.07 | 0.18 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 9 | 0.19 | 0.04 | 0.19 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 9 | 0.19 | 0.04 | 0.19 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 9 | 0.18 | 0.03 | 0.18 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 9 | 0.18 | 0.03 | 0.18 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 9 | 0.17 | 0.04 | 0.16 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 9 | 0.17 | 0.04 | 0.16 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 9 | 0.17 | 0.04 | 0.16 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 9 | 0.16 | 0.03 | 0.17 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 9 | 0.16 | 0.03 | 0.17 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 9 | 0.16 | 0.04 | 0.15 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 9 | 0.15 | 0.04 | 0.13 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 9 | 0.15 | 0.04 | 0.13 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 9 | 0.15 | 0.03 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 9 | 0.15 | 0.03 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 9 | 0.15 | 0.03 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 9 | 0.15 | 0.03 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 9 | 0.15 | 0.03 | 0.14 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 9 | 0.14 | 0.02 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 9 | 0.14 | 0.02 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 9 | 0.14 | 0.02 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 9 | 0.14 | 0.02 | 0.14 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 9 | 0.14 | 0.01 | 0.14 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 9 | 0.13 | 0.02 | 0.13 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 9 | 0.13 | 0.02 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 9 | 0.13 | 0.02 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 9 | 0.13 | 0.02 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 9 | 0.13 | 0.01 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 9 | 0.13 | 0.01 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 9 | 0.13 | 0.01 | 0.12 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 9 | 0.12 | 0.01 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 9 | 0.12 | 0.01 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 9 | 0.12 | 0.01 | 0.12 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 9 | 0.12 | 0.01 | 0.12 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 9 | 0.12 | 0.01 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 9 | 0.12 | 0.01 | 0.11 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 8 | 1.05 | 0.36 | 1.26 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 8 | 1.05 | 0.36 | 1.26 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 8 | 1.05 | 0.36 | 1.26 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 8 | 0.73 | 0.03 | 0.74 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 8 | 0.73 | 0.03 | 0.74 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 8 | 0.67 | 0.4 | 0.55 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 8 | 0.67 | 0.4 | 0.55 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 8 | 0.67 | 0.4 | 0.55 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 8 | 0.66 | 0.03 | 0.66 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 8 | 0.66 | 0.03 | 0.66 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 8 | 0.59 | 0.35 | 0.48 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 8 | 0.59 | 0.35 | 0.48 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 8 | 0.46 | 0.03 | 0.46 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 8 | 0.46 | 0.03 | 0.46 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 8 | 0.42 | 0.22 | 0.42 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 8 | 0.42 | 0.22 | 0.42 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 8 | 0.42 | 0.22 | 0.42 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 8 | 0.42 | 0.22 | 0.42 |
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 8 | 0.42 | 0.22 | 0.41 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 8 | 0.42 | 0.22 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 8 | 0.42 | 0.22 | 0.41 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 8 | 0.42 | 0.22 | 0.41 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 8 | 0.35 | 0.21 | 0.34 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 8 | 0.35 | 0.21 | 0.34 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 8 | 0.35 | 0.21 | 0.34 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 8 | 0.35 | 0.21 | 0.34 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 8 | 0.35 | 0.21 | 0.34 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 8 | 0.35 | 0.21 | 0.34 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 8 | 0.35 | 0.21 | 0.34 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 8 | 0.34 | 0.02 | 0.34 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 8 | 0.31 | 0.08 | 0.32 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 8 | 0.3 | 0.02 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 8 | 0.3 | 0.02 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 8 | 0.3 | 0.02 | 0.3 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 8 | 0.29 | 0.04 | 0.28 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 8 | 0.29 | 0.04 | 0.28 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 8 | 0.25 | 0.03 | 0.26 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 8 | 0.25 | 0.03 | 0.26 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 8 | 0.25 | 0.03 | 0.26 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 8 | 0.24 | 0.02 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 8 | 0.24 | 0.02 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 8 | 0.24 | 0.02 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 8 | 0.24 | 0.02 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 8 | 0.24 | 0.02 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 8 | 0.24 | 0.02 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 8 | 0.22 | 0.06 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 8 | 0.22 | 0.06 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 8 | 0.22 | 0.06 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 8 | 0.22 | 0.06 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 8 | 0.22 | 0.06 | 0.24 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 8 | 0.21 | 0.05 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 8 | 0.21 | 0.05 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 8 | 0.21 | 0.05 | 0.21 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 8 | 0.21 | 0.05 | 0.22 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 8 | 0.21 | 0.05 | 0.22 |
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 8 | 0.21 | 0.05 | 0.22 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 8 | 0.2 | 0.05 | 0.22 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 8 | 0.2 | 0.05 | 0.22 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 8 | 0.2 | 0.03 | 0.2 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 8 | 0.19 | 0.05 | 0.19 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 8 | 0.19 | 0.04 | 0.18 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 8 | 0.18 | 0.02 | 0.18 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 8 | 0.18 | 0.02 | 0.18 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 8 | 0.18 | 0.02 | 0.18 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 8 | 0.18 | 0.02 | 0.18 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 8 | 0.18 | 0.02 | 0.18 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 8 | 0.18 | 0.02 | 0.18 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 8 | 0.18 | 0.02 | 0.18 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 8 | 0.18 | 0.02 | 0.18 |
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 8 | 0.18 | 0.02 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 8 | 0.18 | 0.01 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 8 | 0.18 | 0.01 | 0.18 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 8 | 0.18 | 0.03 | 0.17 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 8 | 0.17 | 0.02 | 0.16 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 8 | 0.16 | 0.03 | 0.16 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 8 | 0.14 | 0.05 | 0.12 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 8 | 0.14 | 0.05 | 0.12 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 8 | 0.14 | 0.02 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 8 | 0.14 | 0.02 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 8 | 0.14 | 0.02 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 8 | 0.14 | 0.01 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 8 | 0.14 | 0.01 | 0.14 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 8 | 0.14 | 0.02 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 8 | 0.14 | 0.02 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 8 | 0.14 | 0.02 | 0.13 |
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 8 | 0.13 | 0.02 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 8 | 0.13 | 0.02 | 0.14 |
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 8 | 0.13 | 0.01 | 0.13 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 8 | 0.13 | 0.01 | 0.12 |
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 8 | 0.13 | 0.01 | 0.12 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 8 | 0.12 | 0.01 | 0.12 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 8 | 0.12 | 0.01 | 0.12 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 8 | 0.12 | 0.01 | 0.12 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 7 | 0.78 | 0.1 | 0.84 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 7 | 0.78 | 0.1 | 0.84 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 7 | 0.78 | 0.1 | 0.84 |
| (2,752) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 7 | 0.78 | 0.1 | 0.84 |
| (2,1936) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 7 | 0.73 | 0.32 | 0.86 |
| (2,1936) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 7 | 0.73 | 0.32 | 0.86 |
| (2,1936) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 7 | 0.73 | 0.32 | 0.86 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 7 | 0.69 | 0.12 | 0.72 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 7 | 0.69 | 0.12 | 0.72 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 7 | 0.69 | 0.12 | 0.72 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 7 | 0.69 | 0.12 | 0.72 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 7 | 0.69 | 0.12 | 0.72 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 7 | 0.69 | 0.12 | 0.72 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 7 | 0.69 | 0.12 | 0.72 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 7 | 0.69 | 0.12 | 0.72 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 7 | 0.69 | 0.12 | 0.72 |
| (2,2580) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 7 | 0.64 | 0.1 | 0.7 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 7 | 0.64 | 0.1 | 0.7 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 7 | 0.64 | 0.1 | 0.7 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 7 | 0.64 | 0.1 | 0.7 |
| (2,795) | 2:B:104:VAL:HG12 | 2:B:103:TYR:HA | 7 | 0.48 | 0.07 | 0.46 |
| (2,795) | 2:B:104:VAL:HG11 | 2:B:103:TYR:HA | 7 | 0.48 | 0.07 | 0.46 |
| (2,795) | 2:B:104:VAL:HG13 | 2:B:103:TYR:HA | 7 | 0.48 | 0.07 | 0.46 |
| (2,795) | 2:B:104:VAL:HG22 | 2:B:103:TYR:HA | 7 | 0.48 | 0.07 | 0.46 |
| (2,3841) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 7 | 0.44 | 0.01 | 0.44 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD11 | 7 | 0.36 | 0.1 | 0.39 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD13 | 7 | 0.36 | 0.1 | 0.39 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD11 | 7 | 0.36 | 0.1 | 0.39 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD13 | 7 | 0.36 | 0.1 | 0.39 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG12 | 7 | 0.29 | 0.06 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG11 | 7 | 0.29 | 0.06 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG13 | 7 | 0.29 | 0.06 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG22 | 7 | 0.29 | 0.06 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG23 | 7 | 0.29 | 0.06 | 0.3 |
| (2,3430) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 7 | 0.28 | 0.13 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 7 | 0.28 | 0.13 | 0.27 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 7 | 0.28 | 0.13 | 0.27 |
| (2,558) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 7 | 0.25 | 0.09 | 0.26 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 7 | 0.25 | 0.09 | 0.26 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 7 | 0.25 | 0.09 | 0.26 |
| (2,4556) | 2:B:161:LYS:HA | 2:B:161:LYS:H | 7 | 0.22 | 0.03 | 0.23 |
| (2,3840) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 7 | 0.19 | 0.01 | 0.19 |
| (2,4119) | 2:B:155:ILE:HB | 2:B:152:GLU:HA | 7 | 0.19 | 0.04 | 0.2 |
| (2,3999) | 2:B:160:GLY:H | 2:B:162:LEU:H | 7 | 0.18 | 0.04 | 0.17 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG22 | 7 | 0.18 | 0.04 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG21 | 7 | 0.18 | 0.04 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG23 | 7 | 0.18 | 0.04 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD21 | 7 | 0.18 | 0.04 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD23 | 7 | 0.18 | 0.04 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG22 | 7 | 0.18 | 0.04 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG21 | 7 | 0.18 | 0.04 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG23 | 7 | 0.18 | 0.04 | 0.16 |
| (2,4509) | 2:B:142:VAL:HB | 2:B:143:ILE:H | 7 | 0.17 | 0.03 | 0.18 |
| (1,82) | 2:B:129:SER:H | 2:B:125:LYS:O | 7 | 0.14 | 0.02 | 0.13 |
| (1,19) | 1:A:16:LEU:N | 1:A:12:SER:O | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD22 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD21 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD23 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD22 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD21 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD23 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD22 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD21 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD23 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD22 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD21 | 7 | 0.13 | 0.02 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD23 | 7 | 0.13 | 0.02 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD12 | 7 | 0.13 | 0.01 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD11 | 7 | 0.13 | 0.01 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD13 | 7 | 0.13 | 0.01 | 0.13 |
| (2,4098) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 7 | 0.13 | 0.02 | 0.12 |
| (2,829) | 2:B:108:LEU:HD12 | 2:B:154:VAL:HB | 7 | 0.12 | 0.01 | 0.12 |
| (2,829) | 2:B:108:LEU:HD13 | 2:B:154:VAL:HB | 7 | 0.12 | 0.01 | 0.12 |
| (2,3668) | 1:A:37:VAL:H | 1:A:37:VAL:HB | 7 | 0.12 | 0.0 | 0.12 |
| (2,4514) | 2:B:144:SER:H | 2:B:143:ILE:HA | 7 | 0.11 | 0.0 | 0.11 |
| (2,3857) | 2:B:125:LYS:H | 2:B:125:LYS:HE3 | 6 | 0.71 | 0.08 | 0.74 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 6 | 0.59 | 0.14 | 0.62 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2626) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 6 | 0.59 | 0.14 | 0.62 |
| (2,2626) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 6 | 0.59 | 0.14 | 0.62 |
| (2,2626) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 6 | 0.59 | 0.14 | 0.62 |
| (2,695) | 1:A:51:LEU:HD12 | 1:A:48:ALA:HA | 6 | 0.54 | 0.89 | 0.15 |
| (2,695) | 1:A:51:LEU:HD11 | 1:A:48:ALA:HA | 6 | 0.54 | 0.89 | 0.15 |
| (2,695) | 1:A:51:LEU:HD13 | 1:A:48:ALA:HA | 6 | 0.54 | 0.89 | 0.15 |
| (2,4521) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 6 | 0.53 | 0.15 | 0.48 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB3 | 6 | 0.46 | 0.23 | 0.48 |
| (2,1994) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HB3 | 6 | 0.46 | 0.23 | 0.48 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB2 | 6 | 0.46 | 0.23 | 0.48 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG22 | 6 | 0.43 | 0.24 | 0.32 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG21 | 6 | 0.43 | 0.24 | 0.32 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG23 | 6 | 0.43 | 0.24 | 0.32 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG12 | 6 | 0.43 | 0.24 | 0.32 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG11 | 6 | 0.43 | 0.24 | 0.32 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG22 | 6 | 0.43 | 0.24 | 0.32 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG21 | 6 | 0.43 | 0.24 | 0.32 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG23 | 6 | 0.43 | 0.24 | 0.32 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 6 | 0.25 | 0.05 | 0.24 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 6 | 0.25 | 0.05 | 0.24 |
| (2,2979) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 6 | 0.25 | 0.05 | 0.24 |
| (2,2979) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 6 | 0.25 | 0.05 | 0.24 |
| (2,2703) | 2:B:109:LEU:HD12 | 2:B:109:LEU:H | 6 | 0.24 | 0.15 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD13 | 2:B:109:LEU:H | 6 | 0.24 | 0.15 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD22 | 2:B:109:LEU:H | 6 | 0.24 | 0.15 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD21 | 2:B:109:LEU:H | 6 | 0.24 | 0.15 | 0.22 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 6 | 0.24 | 0.01 | 0.24 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 6 | 0.24 | 0.01 | 0.24 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 6 | 0.24 | 0.01 | 0.24 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 6 | 0.24 | 0.01 | 0.24 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD11 | 6 | 0.21 | 0.05 | 0.24 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD13 | 6 | 0.21 | 0.05 | 0.24 |
| (2,1132) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 6 | 0.21 | 0.05 | 0.24 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD21 | 6 | 0.21 | 0.05 | 0.24 |
| (2,1132) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 6 | 0.21 | 0.05 | 0.24 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD12 | 6 | 0.21 | 0.05 | 0.24 |
| (2,1132) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 6 | 0.21 | 0.05 | 0.24 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG2 | 6 | 0.19 | 0.06 | 0.2 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG3 | 6 | 0.19 | 0.06 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG12 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG13 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD2 | 6 | 0.19 | 0.04 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD3 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG12 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG13 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HD3 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:151:ILE:HG12 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HD3 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG12 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG13 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:155:ILE:HG12 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG12 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG13 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HD3 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG12 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG13 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HD3 | 6 | 0.19 | 0.04 | 0.2 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 6 | 0.19 | 0.05 | 0.18 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 6 | 0.19 | 0.05 | 0.18 |
| (2,587) | 1:A:37:VAL:HG12 | 2:B:112:LEU:HD23 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD22 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD21 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD21 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 6 | 0.17 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 6 | 0.17 | 0.03 | 0.16 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 6 | 0.17 | 0.03 | 0.16 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB2 | 6 | 0.16 | 0.02 | 0.16 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB3 | 6 | 0.16 | 0.02 | 0.16 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB2 | 6 | 0.16 | 0.02 | 0.16 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB3 | 6 | 0.16 | 0.02 | 0.16 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG2 | 6 | 0.16 | 0.02 | 0.16 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG3 | 6 | 0.16 | 0.02 | 0.16 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD13 | 6 | 0.15 | 0.02 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD22 | 6 | 0.15 | 0.02 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD21 | 6 | 0.15 | 0.02 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD23 | 6 | 0.15 | 0.02 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG12 | 6 | 0.14 | 0.01 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG11 | 6 | 0.14 | 0.01 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG13 | 6 | 0.14 | 0.01 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG21 | 6 | 0.14 | 0.01 | 0.15 |
| (2,4104) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 6 | 0.14 | 0.02 | 0.13 |
| (2,4512) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 6 | 0.14 | 0.02 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD13 | 2:B:159:ILE:HA | 6 | 0.14 | 0.02 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD22 | 2:B:159:ILE:HA | 6 | 0.14 | 0.02 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD21 | 2:B:159:ILE:HA | 6 | 0.14 | 0.02 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD23 | 2:B:159:ILE:HA | 6 | 0.14 | 0.02 | 0.13 |
| (2,4136) | 1:A:22:THR:HA | 1:A:22:THR:HB | 6 | 0.13 | 0.01 | 0.13 |
| (1,87) | 2:B:142:VAL:N | 2:B:138:ARG:O | 6 | 0.13 | 0.01 | 0.12 |
| (2,2589) | 1:A:62:ASN:HB3 | 1:A:43:TRP:HZ2 | 6 | 0.13 | 0.01 | 0.12 |
| (2,2589) | 1:A:62:ASN:HB2 | 1:A:43:TRP:HZ2 | 6 | 0.13 | 0.01 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG22 | 6 | 0.12 | 0.02 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG21 | 6 | 0.12 | 0.02 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG23 | 6 | 0.12 | 0.02 | 0.12 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD12 | 6 | 0.12 | 0.01 | 0.12 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD11 | 6 | 0.12 | 0.01 | 0.12 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD13 | 6 | 0.12 | 0.01 | 0.12 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG22 | 6 | 0.11 | 0.0 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG21 | 6 | 0.11 | 0.0 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG23 | 6 | 0.11 | 0.0 | 0.11 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 5 | 0.78 | 0.04 | 0.8 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 5 | 0.78 | 0.04 | 0.8 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 5 | 0.78 | 0.04 | 0.8 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 5 | 0.78 | 0.04 | 0.8 |
| (2,1063) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 5 | 0.78 | 0.04 | 0.8 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 5 | 0.66 | 0.04 | 0.66 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 5 | 0.66 | 0.04 | 0.66 |
| (2,4458) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 5 | 0.45 | 0.16 | 0.52 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 5 | 0.41 | 0.04 | 0.41 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 5 | 0.41 | 0.04 | 0.41 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 5 | 0.41 | 0.04 | 0.41 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 5 | 0.41 | 0.04 | 0.41 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.39 | 0.07 | 0.37 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.39 | 0.07 | 0.37 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.39 | 0.07 | 0.37 |
| (2,1391) | 1:A:24:THR:HG21 | 1:A:27:LYS:HE3 | 5 | 0.39 | 0.44 | 0.18 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE2 | 5 | 0.39 | 0.44 | 0.18 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE3 | 5 | 0.39 | 0.44 | 0.18 |
| (2,1391) | 1:A:24:THR:HG23 | 1:A:27:LYS:HE3 | 5 | 0.39 | 0.44 | 0.18 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 5 | 0.38 | 0.22 | 0.53 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 5 | 0.38 | 0.22 | 0.53 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 5 | 0.38 | 0.22 | 0.53 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 5 | 0.38 | 0.22 | 0.53 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.38 | 0.07 | 0.36 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.38 | 0.07 | 0.36 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.38 | 0.07 | 0.36 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.3 | 0.07 | 0.28 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.3 | 0.07 | 0.28 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.3 | 0.07 | 0.28 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.28 | 0.07 | 0.26 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.28 | 0.07 | 0.26 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.28 | 0.07 | 0.26 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 5 | 0.25 | 0.05 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 5 | 0.25 | 0.05 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 5 | 0.25 | 0.05 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 5 | 0.25 | 0.05 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 5 | 0.25 | 0.05 | 0.27 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.25 | 0.07 | 0.23 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.25 | 0.07 | 0.23 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.25 | 0.07 | 0.23 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.25 | 0.07 | 0.23 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.25 | 0.07 | 0.23 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.25 | 0.07 | 0.23 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 5 | 0.24 | 0.02 | 0.25 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 5 | 0.24 | 0.02 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 5 | 0.24 | 0.02 | 0.25 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 5 | 0.24 | 0.02 | 0.25 |
| (2,4520) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 5 | 0.22 | 0.14 | 0.15 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 5 | 0.22 | 0.04 | 0.22 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 5 | 0.22 | 0.04 | 0.22 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 5 | 0.22 | 0.04 | 0.22 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 5 | 0.22 | 0.04 | 0.22 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG22 | 5 | 0.21 | 0.06 | 0.21 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG21 | 5 | 0.21 | 0.06 | 0.21 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG21 | 5 | 0.21 | 0.06 | 0.21 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG23 | 5 | 0.21 | 0.06 | 0.21 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE2 | 5 | 0.21 | 0.07 | 0.24 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE3 | 5 | 0.21 | 0.07 | 0.24 |
| (2,1716) | 2:B:121:LYS:HG3 | 2:B:121:LYS:HE3 | 5 | 0.21 | 0.07 | 0.24 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.21 | 0.07 | 0.19 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.21 | 0.07 | 0.19 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.21 | 0.07 | 0.19 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 5 | 0.21 | 0.04 | 0.21 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 5 | 0.21 | 0.04 | 0.21 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 5 | 0.21 | 0.04 | 0.21 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 5 | 0.21 | 0.04 | 0.21 |
| (2,1393) | 1:A:24:THR:HG21 | 1:A:26:ASP:HB3 | 5 | 0.2 | 0.11 | 0.15 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB2 | 5 | 0.2 | 0.11 | 0.15 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB3 | 5 | 0.2 | 0.11 | 0.15 |
| (2,1393) | 1:A:24:THR:HG23 | 1:A:26:ASP:HB3 | 5 | 0.2 | 0.11 | 0.15 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 5 | 0.2 | 0.04 | 0.2 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 5 | 0.2 | 0.04 | 0.2 |
| (2,2328) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 5 | 0.2 | 0.04 | 0.2 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 5 | 0.19 | 0.02 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 5 | 0.19 | 0.02 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 5 | 0.19 | 0.02 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 5 | 0.19 | 0.02 | 0.19 |
| (2,3416) | 2:B:101:MET:HE2 | 1:A:17:HIS:HD2 | 5 | 0.19 | 0.04 | 0.17 |
| (2,3416) | 2:B:101:MET:HE1 | 1:A:17:HIS:HD2 | 5 | 0.19 | 0.04 | 0.17 |
| (2,3416) | 2:B:101:MET:HE3 | 1:A:17:HIS:HD2 | 5 | 0.19 | 0.04 | 0.17 |
| (2,3492) | 2:B:152:GLU:HG2 | 1:A:7:LEU:HB3 | 5 | 0.18 | 0.04 | 0.18 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB2 | 5 | 0.18 | 0.04 | 0.18 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB3 | 5 | 0.18 | 0.04 | 0.18 |
| (2,3347) | 1:A:15:ILE:HG22 | 2:B:101:MET:HE2 | 5 | 0.16 | 0.03 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE2 | 5 | 0.16 | 0.03 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE3 | 5 | 0.16 | 0.03 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE2 | 5 | 0.16 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE1 | 5 | 0.16 | 0.03 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE3 | 5 | 0.16 | 0.03 | 0.16 |
| (2,4251) | 1:A:15:ILE:HA | 2:B:103:TYR:HA | 5 | 0.16 | 0.03 | 0.15 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD12 | 5 | 0.16 | 0.02 | 0.16 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD11 | 5 | 0.16 | 0.02 | 0.16 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD13 | 5 | 0.16 | 0.02 | 0.16 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 5 | 0.15 | 0.02 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 5 | 0.15 | 0.02 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 5 | 0.15 | 0.02 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 5 | 0.15 | 0.02 | 0.15 |
| (2,1614) | 2:B:101:MET:HE1 | 1:A:14:LEU:HB2 | 5 | 0.15 | 0.04 | 0.14 |
| (2,1614) | 2:B:101:MET:HE3 | 1:A:14:LEU:HB2 | 5 | 0.15 | 0.04 | 0.14 |
| (2,1614) | 2:B:101:MET:HE2 | 1:A:14:LEU:HB2 | 5 | 0.15 | 0.04 | 0.14 |
| (1,81) | 2:B:129:SER:N | 2:B:125:LYS:O | 5 | 0.15 | 0.02 | 0.15 |
| (2,1876) | 2:B:143:ILE:HG21 | 2:B:147:ASN:HB2 | 5 | 0.14 | 0.03 | 0.12 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB2 | 5 | 0.14 | 0.03 | 0.12 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB3 | 5 | 0.14 | 0.03 | 0.12 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG2 | 5 | 0.13 | 0.02 | 0.14 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG3 | 5 | 0.13 | 0.02 | 0.14 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG2 | 5 | 0.13 | 0.02 | 0.14 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,13) | 1:A:13:ALA:N | 1:A:9:CYS:O | 5 | 0.13 | 0.02 | 0.12 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB3 | 5 | 0.13 | 0.02 | 0.12 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG22 | 5 | 0.13 | 0.01 | 0.13 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG21 | 5 | 0.13 | 0.01 | 0.13 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG23 | 5 | 0.13 | 0.01 | 0.13 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB3 | 5 | 0.12 | 0.01 | 0.12 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB2 | 5 | 0.12 | 0.01 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG12 | 1:A:51:LEU:H | 5 | 0.12 | 0.01 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG11 | 1:A:51:LEU:H | 5 | 0.12 | 0.01 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG13 | 1:A:51:LEU:H | 5 | 0.12 | 0.01 | 0.12 |
| (1,55) | 2:B:107:TYR:N | 2:B:103:TYR:O | 5 | 0.12 | 0.01 | 0.12 |
| (2,951) | 2:B:125:LYS:HD2 | 2:B:129:SER:HB3 | 4 | 0.82 | 0.26 | 0.84 |
| (2,951) | 2:B:125:LYS:HD3 | 2:B:129:SER:HB3 | 4 | 0.82 | 0.26 | 0.84 |
| (2,3962) | 2:B:144:SER:H | 2:B:143:ILE:HG12 | 4 | 0.8 | 0.02 | 0.8 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 4 | 0.75 | 0.01 | 0.75 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 4 | 0.75 | 0.01 | 0.75 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 4 | 0.68 | 0.01 | 0.68 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 4 | 0.68 | 0.01 | 0.68 |
| (2,4291) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 4 | 0.56 | 0.01 | 0.56 |
| (2,4290) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 4 | 0.53 | 0.01 | 0.54 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 4 | 0.52 | 0.01 | 0.52 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 4 | 0.52 | 0.01 | 0.52 |
| (2,3221) | 2:B:159:ILE:HD12 | 2:B:158:GLY:H | 4 | 0.48 | 0.21 | 0.56 |
| (2,3221) | 2:B:159:ILE:HD13 | 2:B:158:GLY:H | 4 | 0.48 | 0.21 | 0.56 |
| (2,3221) | 2:B:159:ILE:HD12 | 1:A:61:CYS:H | 4 | 0.48 | 0.21 | 0.56 |
| (2,3221) | 2:B:159:ILE:HD13 | 1:A:61:CYS:H | 4 | 0.48 | 0.21 | 0.56 |
| (2,2256) | 1:A:25:GLU:HG3 | 1:A:29:ASN:HD22 | 4 | 0.4 | 0.18 | 0.43 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD21 | 4 | 0.4 | 0.18 | 0.43 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD22 | 4 | 0.4 | 0.18 | 0.43 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 4 | 0.38 | 0.01 | 0.38 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 4 | 0.38 | 0.01 | 0.38 |
| (2,1654) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 4 | 0.35 | 0.09 | 0.35 |
| (2,1654) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 4 | 0.35 | 0.09 | 0.35 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 4 | 0.35 | 0.09 | 0.35 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 4 | 0.35 | 0.09 | 0.35 |
| (2,1809) | 2:B:132:ILE:HG22 | 1:A:18:ASP:HB2 | 4 | 0.35 | 0.14 | 0.34 |
| (2,1809) | 2:B:132:ILE:HG23 | 1:A:18:ASP:HB2 | 4 | 0.35 | 0.14 | 0.34 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD12 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD11 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD13 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD12 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD11 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD13 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD12 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD11 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD13 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD12 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD11 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD13 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD12 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD11 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD13 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD11 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD13 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD11 | 4 | 0.34 | 0.03 | 0.33 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD13 | 4 | 0.34 | 0.03 | 0.33 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG12 | 4 | 0.3 | 0.3 | 0.13 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG13 | 4 | 0.3 | 0.3 | 0.13 |
| (2,3509) | 2:B:159:ILE:HG23 | 1:A:10:ILE:HG13 | 4 | 0.3 | 0.3 | 0.13 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG12 | 4 | 0.3 | 0.3 | 0.13 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG13 | 4 | 0.3 | 0.3 | 0.13 |
| (2,1102) | 2:B:143:ILE:HD12 | 2:B:107:TYR:HD2 | 4 | 0.26 | 0.02 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1102) | 2:B:143:ILE:HD11 | 2:B:107:TYR:HD2 | 4 | 0.26 | 0.02 | 0.25 |
| (2,1102) | 2:B:143:ILE:HD13 | 2:B:107:TYR:HD2 | 4 | 0.26 | 0.02 | 0.25 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD12 | 4 | 0.26 | 0.22 | 0.14 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD11 | 4 | 0.26 | 0.22 | 0.14 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD13 | 4 | 0.26 | 0.22 | 0.14 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD12 | 4 | 0.26 | 0.22 | 0.14 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD11 | 4 | 0.26 | 0.22 | 0.14 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD13 | 4 | 0.26 | 0.22 | 0.14 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD21 | 4 | 0.26 | 0.22 | 0.14 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD23 | 4 | 0.26 | 0.22 | 0.14 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 4 | 0.25 | 0.09 | 0.25 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 4 | 0.25 | 0.09 | 0.25 |
| (2,847) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 4 | 0.25 | 0.09 | 0.25 |
| (2,847) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 4 | 0.25 | 0.09 | 0.25 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD21 | 4 | 0.24 | 0.17 | 0.15 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD22 | 4 | 0.24 | 0.17 | 0.15 |
| (2,2579) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HD21 | 4 | 0.24 | 0.17 | 0.15 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD12 | 4 | 0.22 | 0.02 | 0.22 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD11 | 4 | 0.22 | 0.02 | 0.22 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD13 | 4 | 0.22 | 0.02 | 0.22 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG2 | 4 | 0.21 | 0.03 | 0.2 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG3 | 4 | 0.21 | 0.03 | 0.2 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG2 | 4 | 0.21 | 0.01 | 0.21 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG3 | 4 | 0.21 | 0.01 | 0.21 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 4 | 0.2 | 0.07 | 0.2 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 4 | 0.2 | 0.07 | 0.2 |
| (2,2627) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 4 | 0.2 | 0.07 | 0.2 |
| (2,2627) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 4 | 0.2 | 0.07 | 0.2 |
| (2,569) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 4 | 0.19 | 0.0 | 0.19 |
| (2,569) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 4 | 0.19 | 0.0 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 4 | 0.19 | 0.0 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 4 | 0.19 | 0.0 | 0.19 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD2 | 4 | 0.18 | 0.04 | 0.18 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD3 | 4 | 0.18 | 0.04 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,4517) | 2:B:144:SER:HA | 2:B:143:ILE:HB | 4 | 0.18 | 0.02 | 0.17 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 4 | 0.17 | 0.02 | 0.18 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 4 | 0.17 | 0.02 | 0.18 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG22 | 4 | 0.17 | 0.0 | 0.17 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG21 | 4 | 0.17 | 0.0 | 0.17 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG21 | 4 | 0.16 | 0.03 | 0.16 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG23 | 4 | 0.16 | 0.03 | 0.16 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG2 | 4 | 0.16 | 0.02 | 0.15 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG3 | 4 | 0.16 | 0.02 | 0.15 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB2 | 4 | 0.16 | 0.01 | 0.15 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB3 | 4 | 0.16 | 0.01 | 0.15 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB2 | 4 | 0.15 | 0.03 | 0.14 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB3 | 4 | 0.15 | 0.03 | 0.14 |
| (2,2976) | 2:B:134:ALA:HB2 | 2:B:135:ASP:HB3 | 4 | 0.15 | 0.02 | 0.16 |
| (2,2976) | 2:B:134:ALA:HB1 | 2:B:135:ASP:HB3 | 4 | 0.15 | 0.02 | 0.16 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB2 | 4 | 0.15 | 0.02 | 0.16 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB3 | 4 | 0.15 | 0.02 | 0.16 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG2 | 4 | 0.15 | 0.01 | 0.15 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG3 | 4 | 0.15 | 0.01 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG12 | 2:B:107:TYR:HD2 | 4 | 0.14 | 0.03 | 0.14 |
| (2,3054) | 2:B:142:VAL:HG11 | 2:B:107:TYR:HD2 | 4 | 0.14 | 0.03 | 0.14 |
| (2,3054) | 2:B:142:VAL:HG13 | 2:B:107:TYR:HD2 | 4 | 0.14 | 0.03 | 0.14 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD1 | 4 | 0.14 | 0.03 | 0.14 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD2 | 4 | 0.14 | 0.03 | 0.14 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HE2 | 4 | 0.14 | 0.03 | 0.14 |
| (2,3054) | 2:B:142:VAL:HG21 | 2:B:107:TYR:HD2 | 4 | 0.14 | 0.03 | 0.14 |
| (2,3054) | 2:B:142:VAL:HG23 | 2:B:107:TYR:HD2 | 4 | 0.14 | 0.03 | 0.14 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD12 | 4 | 0.14 | 0.02 | 0.15 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD11 | 4 | 0.14 | 0.02 | 0.15 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD13 | 4 | 0.14 | 0.02 | 0.15 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD21 | 4 | 0.14 | 0.02 | 0.15 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 4 | 0.14 | 0.01 | 0.15 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 4 | 0.14 | 0.01 | 0.15 |
| (2,850) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 4 | 0.14 | 0.01 | 0.15 |
| (2,850) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 4 | 0.14 | 0.01 | 0.15 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 4 | 0.14 | 0.02 | 0.15 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 4 | 0.14 | 0.02 | 0.15 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 4 | 0.14 | 0.02 | 0.15 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 4 | 0.14 | 0.02 | 0.15 |
| (1,75) | 2:B:126:ILE:N | 2:B:122:ASP:O | 4 | 0.14 | 0.02 | 0.14 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB2 | 4 | 0.14 | 0.01 | 0.14 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB3 | 4 | 0.14 | 0.01 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB1 | 4 | 0.14 | 0.02 | 0.13 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB3 | 4 | 0.14 | 0.02 | 0.13 |
| (2,4393) | 1:A:63:VAL:HA | 1:A:64:GLY:H | 4 | 0.14 | 0.04 | 0.12 |
| (2,3954) | 2:B:143:ILE:H | 2:B:107:TYR:HE2 | 4 | 0.13 | 0.02 | 0.12 |
| (2,1988) | 2:B:161:LYS:HD2 | 2:B:161:LYS:HA | 4 | 0.13 | 0.01 | 0.13 |
| (2,1988) | 2:B:161:LYS:HD3 | 2:B:161:LYS:HA | 4 | 0.13 | 0.01 | 0.13 |
| (2,3783) | 2:B:108:LEU:H | 2:B:108:LEU:HG | 4 | 0.12 | 0.01 | 0.12 |
| (2,4341) | 1:A:41:PRO:HA | 1:A:39:VAL:H | 4 | 0.12 | 0.01 | 0.12 |
| (2,4522) | 2:B:146:LEU:HA | 2:B:146:LEU:HG | 4 | 0.12 | 0.0 | 0.12 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 4 | 0.11 | 0.0 | 0.11 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 4 | 0.11 | 0.0 | 0.11 |
| (2,4503) | 2:B:140:ASN:HA | 2:B:141:LYS:H | 4 | 0.11 | 0.0 | 0.11 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB2 | 3 | 0.91 | 0.12 | 0.98 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB1 | 3 | 0.91 | 0.12 | 0.98 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB3 | 3 | 0.91 | 0.12 | 0.98 |
| (2,2583) | 1:A:61:CYS:HB3 | 1:A:65:ALA:HB3 | 3 | 0.91 | 0.12 | 0.98 |
| (2,3739) | 1:A:59:LEU:H | 1:A:58:SER:HB3 | 3 | 0.83 | 0.03 | 0.83 |
| (2,2318) | 1:A:32:ILE:HD12 | 1:A:9:CYS:H | 3 | 0.74 | 0.04 | 0.73 |
| (2,2318) | 1:A:32:ILE:HD13 | 1:A:9:CYS:H | 3 | 0.74 | 0.04 | 0.73 |
| (2,1060) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HD2 | 3 | 0.73 | 0.42 | 0.65 |
| (2,1060) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HD2 | 3 | 0.73 | 0.42 | 0.65 |
| (2,1060) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HD2 | 3 | 0.73 | 0.42 | 0.65 |
| (2,1594) | 1:A:60:ILE:HD12 | 1:A:60:ILE:HG22 | 3 | 0.72 | 0.0 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HG22 | 3 | 0.72 | 0.0 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HG21 | 3 | 0.72 | 0.0 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG22 | 3 | 0.72 | 0.0 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG21 | 3 | 0.72 | 0.0 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG23 | 3 | 0.72 | 0.0 | 0.72 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 3 | 0.54 | 0.02 | 0.54 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 3 | 0.54 | 0.02 | 0.54 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 3 | 0.54 | 0.02 | 0.54 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 3 | 0.54 | 0.02 | 0.54 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 3 | 0.45 | 0.02 | 0.45 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 3 | 0.45 | 0.02 | 0.45 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 3 | 0.45 | 0.02 | 0.45 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 3 | 0.45 | 0.02 | 0.45 |
| (2,792) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 3 | 0.45 | 0.23 | 0.51 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 3 | 0.45 | 0.23 | 0.51 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 3 | 0.45 | 0.23 | 0.51 |
| (2,3017) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 3 | 0.43 | 0.07 | 0.44 |
| (2,3017) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 3 | 0.43 | 0.07 | 0.44 |
| (2,3017) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 3 | 0.43 | 0.07 | 0.44 |
| (2,3017) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 3 | 0.43 | 0.07 | 0.44 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 3 | 0.4 | 0.02 | 0.4 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 3 | 0.4 | 0.02 | 0.4 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 3 | 0.4 | 0.02 | 0.4 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 3 | 0.4 | 0.02 | 0.4 |
| (2,1059) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 3 | 0.37 | 0.07 | 0.38 |
| (2,1059) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 3 | 0.37 | 0.07 | 0.38 |
| (2,1059) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 3 | 0.37 | 0.07 | 0.38 |
| (2,1059) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 3 | 0.37 | 0.07 | 0.38 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 3 | 0.34 | 0.02 | 0.34 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 3 | 0.34 | 0.02 | 0.34 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 3 | 0.34 | 0.02 | 0.34 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 3 | 0.34 | 0.02 | 0.34 |
| (2,1598) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 3 | 0.31 | 0.07 | 0.27 |
| (2,1598) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 3 | 0.31 | 0.07 | 0.27 |
| (2,1598) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 3 | 0.31 | 0.07 | 0.27 |
| (2,1598) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 3 | 0.31 | 0.07 | 0.27 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB2 | 3 | 0.29 | 0.02 | 0.29 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB1 | 3 | 0.29 | 0.02 | 0.29 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB3 | 3 | 0.29 | 0.02 | 0.29 |
| (2,493) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB1 | 3 | 0.29 | 0.02 | 0.29 |
| (2,493) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB3 | 3 | 0.29 | 0.02 | 0.29 |
| (2,522) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 3 | 0.27 | 0.13 | 0.23 |
| (2,522) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 3 | 0.27 | 0.13 | 0.23 |
| (2,1510) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 3 | 0.27 | 0.13 | 0.23 |
| (2,1510) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 3 | 0.27 | 0.13 | 0.23 |
| (2,2286) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 3 | 0.27 | 0.13 | 0.23 |
| (2,2286) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 3 | 0.27 | 0.13 | 0.23 |
| (2,1700) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 3 | 0.23 | 0.07 | 0.24 |
| (2,1700) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 3 | 0.23 | 0.07 | 0.24 |
| (2,1700) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 3 | 0.23 | 0.07 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (2,1700) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 3 | 0.23 | 0.07 | 0.24 |
| (2,325) | 2:B:161:LYS:H | 2:B:161:LYS:HB2 | 3 | 0.22 | 0.01 | 0.23 |
| (2,325) | 2:B:161:LYS:H | 2:B:161:LYS:HB3 | 3 | 0.22 | 0.01 | 0.23 |
| (2,327) | 2:B:162:LEU:H | 2:B:162:LEU:HB2 | 3 | 0.22 | 0.01 | 0.22 |
| (2,327) | 2:B:162:LEU:H | 2:B:162:LEU:HB3 | 3 | 0.22 | 0.01 | 0.22 |
| (2,3247) | 2:B:162:LEU:H | 2:B:162:LEU:HB2 | 3 | 0.22 | 0.01 | 0.22 |
| (2,3247) | 2:B:162:LEU:H | 2:B:162:LEU:HB3 | 3 | 0.22 | 0.01 | 0.22 |
| (2,1721) | 2:B:122:ASP:HA | 2:B:125:LYS:HG2 | 3 | 0.19 | 0.07 | 0.18 |
| (2,1721) | 2:B:122:ASP:HA | 2:B:125:LYS:HG3 | 3 | 0.19 | 0.07 | 0.18 |
| (2,1989) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 3 | 0.19 | 0.01 | 0.19 |
| (2,1989) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 3 | 0.19 | 0.01 | 0.19 |
| (2,282) | 2:B:140:ASN:H | 2:B:141:LYS:HB2 | 3 | 0.18 | 0.06 | 0.17 |
| (2,282) | 2:B:140:ASN:H | 2:B:141:LYS:HB3 | 3 | 0.18 | 0.06 | 0.17 |
| (2,1219) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 3 | 0.18 | 0.01 | 0.18 |
| (2,1219) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 3 | 0.18 | 0.01 | 0.18 |
| (2,1034) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 3 | 0.17 | 0.03 | 0.17 |
| (2,1034) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 3 | 0.17 | 0.03 | 0.17 |
| (2,1034) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 3 | 0.17 | 0.03 | 0.17 |
| (2,1034) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 3 | 0.17 | 0.03 | 0.17 |
| (2,3237) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 3 | 0.16 | 0.01 | 0.16 |
| (2,3237) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 3 | 0.16 | 0.01 | 0.16 |
| (2,3010) | 2:B:138:ARG:HG2 | 2:B:135:ASP:H | 3 | 0.16 | 0.03 | 0.16 |
| (2,3010) | 2:B:138:ARG:HG3 | 2:B:135:ASP:H | 3 | 0.16 | 0.03 | 0.16 |
| (2,739) | 1:A:59:LEU:HD12 | 1:A:56:ILE:HA | 3 | 0.15 | 0.04 | 0.13 |
| (2,739) | 1:A:59:LEU:HD11 | 1:A:56:ILE:HA | 3 | 0.15 | 0.04 | 0.13 |
| (2,739) | 1:A:59:LEU:HD13 | 1:A:56:ILE:HA | 3 | 0.15 | 0.04 | 0.13 |
| (2,739) | 1:A:59:LEU:HD21 | 1:A:56:ILE:HA | 3 | 0.15 | 0.04 | 0.13 |
| (2,1601) | 1:A:61:CYS:HA | 1:A:61:CYS:HB2 | 3 | 0.13 | 0.0 | 0.13 |
| (2,1601) | 1:A:61:CYS:HA | 1:A:61:CYS:HB3 | 3 | 0.13 | 0.0 | 0.13 |
| (2,2607) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD2 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD2 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD1 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD11 | 1:A:47:PHE:HD1 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD1 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD13 | 1:A:47:PHE:HD1 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD23 | 1:A:47:PHE:HD2 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD13 | 1:A:47:PHE:HD2 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD23 | 1:A:47:PHE:HD1 | 3 | 0.13 | 0.01 | 0.14 |
| (2,2716) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 3 | 0.13 | 0.01 | 0.13 |
| (2,2716) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 3 | 0.13 | 0.01 | 0.13 |
| (2,2716) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 3 | 0.13 | 0.01 | 0.13 |
| (2,2716) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 3 | 0.13 | 0.01 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (2,4446) | 2:B:120:ALA:HA | 2:B:140:ASN:HA | 3 | 0.13 | 0.01 | 0.12 |
| (1,32) | 1:A:31:LEU:H | 1:A:27:LYS:O | 3 | 0.13 | 0.01 | 0.12 |
| (2,296) | 2:B:144:SER:H | 2:B:141:LYS:HG2 | 3 | 0.13 | 0.02 | 0.11 |
| (2,296) | 2:B:144:SER:H | 2:B:141:LYS:HG3 | 3 | 0.13 | 0.02 | 0.11 |
| (2,3728) | 1:A:55:ASN:H | 1:A:54:VAL:H | 3 | 0.13 | 0.02 | 0.12 |
| (2,1191) | 2:B:157:GLN:HB2 | 2:B:154:VAL:HA | 3 | 0.12 | 0.0 | 0.12 |
| (2,1191) | 2:B:157:GLN:HB3 | 2:B:154:VAL:HA | 3 | 0.12 | 0.0 | 0.12 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG12 | 3 | 0.12 | 0.01 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG11 | 3 | 0.12 | 0.01 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG13 | 3 | 0.12 | 0.01 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG23 | 3 | 0.12 | 0.01 | 0.11 |
| (2,4046) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 3 | 0.12 | 0.01 | 0.12 |
| (1,6) | 1:A:9:CYS:H | 1:A:5:SER:O | 3 | 0.11 | 0.0 | 0.11 |
| (2,617) | 1:A:40:GLU:HG2 | 1:A:40:GLU:HA | 3 | 0.11 | 0.0 | 0.11 |
| (2,617) | 1:A:40:GLU:HG3 | 1:A:40:GLU:HA | 3 | 0.11 | 0.0 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 3 | 0.11 | 0.0 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 3 | 0.11 | 0.0 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 3 | 0.11 | 0.0 | 0.11 |
| (2,1225) | 2:B:162:LEU:HB2 | 2:B:162:LEU:HG | 3 | 0.11 | 0.0 | 0.11 |
| (2,1225) | 2:B:162:LEU:HB3 | 2:B:162:LEU:HG | 3 | 0.11 | 0.0 | 0.11 |
| (2,2417) | 1:A:40:GLU:HG2 | 1:A:40:GLU:HA | 3 | 0.11 | 0.0 | 0.11 |
| (2,2417) | 1:A:40:GLU:HG3 | 1:A:40:GLU:HA | 3 | 0.11 | 0.0 | 0.11 |
| (2,2368) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 2 | 0.84 | 0.05 | 0.84 |
| (2,2368) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 2 | 0.84 | 0.05 | 0.84 |
| (2,2368) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 2 | 0.84 | 0.05 | 0.84 |
| (2,2368) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 2 | 0.84 | 0.05 | 0.84 |
| (2,2368) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 2 | 0.84 | 0.05 | 0.84 |
| (2,596) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 2 | 0.82 | 0.05 | 0.82 |
| (2,596) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 2 | 0.82 | 0.05 | 0.82 |
| (2,596) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 2 | 0.82 | 0.05 | 0.82 |
| (2,596) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 2 | 0.82 | 0.05 | 0.82 |
| (2,596) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 2 | 0.82 | 0.05 | 0.82 |
| (2,3269) | 2:B:165:VAL:H | 2:B:165:VAL:HG22 | 2 | 0.82 | 0.68 | 0.82 |
| (2,3269) | 2:B:165:VAL:H | 2:B:165:VAL:HG21 | 2 | 0.82 | 0.68 | 0.82 |
| (2,4008) | 1:A:4:VAL:HB | 1:A:3:SER:HB3 | 2 | 0.8 | 0.01 | 0.8 |
| (2,4222) | 1:A:4:VAL:HB | 1:A:3:SER:HB3 | 2 | 0.8 | 0.01 | 0.8 |
| (2,3387) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 2 | 0.73 | 0.05 | 0.73 |
| (2,3387) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 2 | 0.73 | 0.05 | 0.73 |
| (2,3387) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 2 | 0.73 | 0.05 | 0.73 |
| (2,3387) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 2 | 0.73 | 0.05 | 0.73 |
| (2,3387) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 2 | 0.73 | 0.05 | 0.73 |
| (2,4080) | 2:B:122:ASP:HA | 2:B:125:LYS:HB2 | 2 | 0.57 | 0.07 | 0.57 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2861) | 2:B:124:LYS:HE3 | 2:B:124:LYS:HB2 | 2 | 0.55 | 0.44 | 0.55 |
| (2,2861) | 2:B:124:LYS:HE3 | 2:B:124:LYS:HB3 | 2 | 0.55 | 0.44 | 0.55 |
| (2,950) | 2:B:125:LYS:HB2 | 2:B:122:ASP:HB2 | 2 | 0.54 | 0.08 | 0.54 |
| (2,950) | 2:B:125:LYS:HB2 | 2:B:122:ASP:HB3 | 2 | 0.54 | 0.08 | 0.54 |
| (2,4462) | 2:B:125:LYS:H | 2:B:125:LYS:HB2 | 2 | 0.54 | 0.05 | 0.54 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG22 | 2 | 0.49 | 0.03 | 0.49 |
| (2,1945) | 2:B:149:LYS:HB3 | 2:B:154:VAL:HG22 | 2 | 0.49 | 0.03 | 0.49 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG21 | 2 | 0.49 | 0.03 | 0.49 |
| (2,1945) | 2:B:149:LYS:HB3 | 2:B:154:VAL:HG21 | 2 | 0.49 | 0.03 | 0.49 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG23 | 2 | 0.49 | 0.03 | 0.49 |
| (2,4084) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 2 | 0.48 | 0.32 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 2 | 0.48 | 0.09 | 0.48 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 2 | 0.48 | 0.09 | 0.48 |
| (2,3390) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 2 | 0.48 | 0.06 | 0.48 |
| (2,3390) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 2 | 0.48 | 0.06 | 0.48 |
| (2,3390) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 2 | 0.48 | 0.06 | 0.48 |
| (2,3390) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 2 | 0.48 | 0.06 | 0.48 |
| (2,3390) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 2 | 0.48 | 0.06 | 0.48 |
| (2,1105) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD12 | 2 | 0.44 | 0.33 | 0.44 |
| (2,1105) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD13 | 2 | 0.44 | 0.33 | 0.44 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD12 | 2 | 0.44 | 0.33 | 0.44 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD11 | 2 | 0.44 | 0.33 | 0.44 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD13 | 2 | 0.44 | 0.33 | 0.44 |
| (2,3074) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD13 | 2 | 0.44 | 0.33 | 0.44 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD12 | 2 | 0.44 | 0.33 | 0.44 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD11 | 2 | 0.44 | 0.33 | 0.44 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD13 | 2 | 0.44 | 0.33 | 0.44 |
| (2,3074) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD12 | 2 | 0.44 | 0.33 | 0.44 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD11 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD13 | 2 | 0.42 | 0.06 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2742) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD12 | 2:B:108:LEU:HB2 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD11 | 2:B:108:LEU:HB2 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD13 | 2:B:108:LEU:HB2 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD22 | 2:B:109:LEU:HD12 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD22 | 2:B:109:LEU:HD13 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD21 | 2:B:109:LEU:HD12 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD21 | 2:B:109:LEU:HD13 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 2 | 0.42 | 0.06 | 0.42 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD12 | 2 | 0.42 | 0.06 | 0.42 |
| (2,4456) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 2 | 0.42 | 0.22 | 0.42 |
| (2,621) | 1:A:40:GLU:HG2 | 1:A:42:PHE:HE2 | 2 | 0.4 | 0.02 | 0.4 |
| (2,621) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE1 | 2 | 0.4 | 0.02 | 0.4 |
| (2,621) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE2 | 2 | 0.4 | 0.02 | 0.4 |
| (2,2410) | 1:A:40:GLU:HG2 | 1:A:42:PHE:HE2 | 2 | 0.4 | 0.02 | 0.4 |
| (2,2410) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE1 | 2 | 0.4 | 0.02 | 0.4 |
| (2,2410) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE2 | 2 | 0.4 | 0.02 | 0.4 |
| (2,1625) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 2 | 0.39 | 0.09 | 0.39 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 2 | 0.39 | 0.09 | 0.39 |
| (2,2645) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 2 | 0.38 | 0.09 | 0.38 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2645) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 2 | 0.38 | 0.09 | 0.38 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 2 | 0.38 | 0.09 | 0.38 |
| (2,3858) | 2:B:125:LYS:H | 2:B:125:LYS:HB2 | 2 | 0.38 | 0.05 | 0.38 |
| (2,2257) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD21 | 2 | 0.35 | 0.02 | 0.35 |
| (2,2257) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD22 | 2 | 0.35 | 0.02 | 0.35 |
| (2,2257) | 1:A:25:GLU:HG3 | 1:A:29:ASN:HD22 | 2 | 0.35 | 0.02 | 0.35 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD12 | 2 | 0.34 | 0.08 | 0.34 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD13 | 2 | 0.34 | 0.08 | 0.34 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD22 | 2 | 0.34 | 0.08 | 0.34 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 2 | 0.34 | 0.08 | 0.34 |
| (2,1136) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB2 | 2 | 0.34 | 0.08 | 0.34 |
| (2,1136) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB3 | 2 | 0.34 | 0.08 | 0.34 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 2 | 0.34 | 0.08 | 0.34 |
| (2,1765) | 2:B:126:ILE:HD12 | 2:B:125:LYS:HD2 | 2 | 0.32 | 0.06 | 0.32 |
| (2,1765) | 2:B:126:ILE:HD12 | 2:B:125:LYS:HD3 | 2 | 0.32 | 0.06 | 0.32 |
| (2,1765) | 2:B:126:ILE:HD11 | 2:B:125:LYS:HD2 | 2 | 0.32 | 0.06 | 0.32 |
| (2,1765) | 2:B:126:ILE:HD11 | 2:B:125:LYS:HD3 | 2 | 0.32 | 0.06 | 0.32 |
| (2,2373) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 2 | 0.3 | 0.05 | 0.3 |
| (2,2373) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 2 | 0.3 | 0.05 | 0.3 |
| (2,2373) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 2 | 0.3 | 0.05 | 0.3 |
| (2,2373) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 2 | 0.3 | 0.05 | 0.3 |
| (2,2373) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 2 | 0.3 | 0.05 | 0.3 |
| (2,4181) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 2 | 0.3 | 0.0 | 0.3 |
| (2,1540) | 1:A:47:PHE:HA | 1:A:51:LEU:HD12 | 2 | 0.3 | 0.16 | 0.3 |
| (2,1540) | 1:A:47:PHE:HA | 1:A:51:LEU:HD13 | 2 | 0.3 | 0.16 | 0.3 |
| (2,1540) | 1:A:56:ILE:HA | 1:A:51:LEU:HD13 | 2 | 0.3 | 0.16 | 0.3 |
| (2,1540) | 1:A:56:ILE:HA | 1:A:51:LEU:HD23 | 2 | 0.3 | 0.16 | 0.3 |
| (2,3205) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 2 | 0.29 | 0.18 | 0.29 |
| (2,3205) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 2 | 0.29 | 0.18 | 0.29 |
| (2,3205) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 2 | 0.29 | 0.18 | 0.29 |
| (2,3205) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 2 | 0.29 | 0.18 | 0.29 |
| (2,217) | 2:B:117:SER:H | 2:B:115:ASN:HD21 | 2 | 0.28 | 0.01 | 0.28 |
| (2,217) | 2:B:117:SER:H | 2:B:115:ASN:HD22 | 2 | 0.28 | 0.01 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2738) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 2 | 0.26 | 0.01 | 0.26 |
| (2,4391) | 1:A:61:CYS:HA | 1:A:62:ASN:HA | 2 | 0.26 | 0.01 | 0.26 |
| (2,586) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 2 | 0.24 | 0.05 | 0.24 |
| (2,586) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 2 | 0.24 | 0.05 | 0.24 |
| (2,586) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 2 | 0.24 | 0.05 | 0.24 |
| (2,586) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 2 | 0.24 | 0.05 | 0.24 |
| (2,586) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 2 | 0.24 | 0.05 | 0.24 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD12 | 2 | 0.22 | 0.08 | 0.22 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD13 | 2 | 0.22 | 0.08 | 0.22 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD22 | 2 | 0.22 | 0.08 | 0.22 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 2 | 0.22 | 0.08 | 0.22 |
| (2,3111) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB2 | 2 | 0.22 | 0.08 | 0.22 |
| (2,3111) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB3 | 2 | 0.22 | 0.08 | 0.22 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 2 | 0.22 | 0.08 | 0.22 |
| (2,790) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 2 | 0.22 | 0.09 | 0.22 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 2 | 0.22 | 0.09 | 0.22 |
| (2,920) | 2:B:122:ASP:HA | 2:B:125:LYS:HG2 | 2 | 0.2 | 0.06 | 0.2 |
| (2,920) | 2:B:122:ASP:HA | 2:B:125:LYS:HG3 | 2 | 0.2 | 0.06 | 0.2 |
| (2,3385) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 2 | 0.2 | 0.06 | 0.2 |
| (2,3385) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 2 | 0.2 | 0.06 | 0.2 |
| (2,3385) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 2 | 0.2 | 0.06 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (2,3385) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 2 | 0.2 | 0.06 | 0.2 |
| (2,3385) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 2 | 0.2 | 0.06 | 0.2 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG23 | 2 | 0.2 | 0.03 | 0.2 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HD12 | 2 | 0.2 | 0.03 | 0.2 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG23 | 2 | 0.2 | 0.03 | 0.2 |
| (2,567) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (2,567) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG23 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HD12 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG22 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG21 | 2 | 0.2 | 0.03 | 0.2 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG23 | 2 | 0.2 | 0.03 | 0.2 |
| (2,1967) | 2:B:157:GLN:HA | 2:B:157:GLN:HG2 | 2 | 0.2 | 0.02 | 0.2 |
| (2,1967) | 2:B:157:GLN:HA | 2:B:157:GLN:HG3 | 2 | 0.2 | 0.02 | 0.2 |
| (2,159) | 1:A:63:VAL:H | 1:A:62:ASN:HB2 | 2 | 0.19 | 0.04 | 0.19 |
| (2,159) | 1:A:63:VAL:H | 1:A:62:ASN:HB3 | 2 | 0.19 | 0.04 | 0.19 |
| (2,761) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 2 | 0.19 | 0.02 | 0.19 |
| (2,761) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 2 | 0.19 | 0.02 | 0.19 |
| (2,761) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 2 | 0.19 | 0.02 | 0.19 |
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 2 | 0.19 | 0.04 | 0.19 |
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 2 | 0.19 | 0.04 | 0.19 |
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 2 | 0.19 | 0.04 | 0.19 |
| (2,2285) | 1:A:28:ILE:HA | 1:A:31:LEU:HD22 | 2 | 0.18 | 0.04 | 0.18 |
| (2,2285) | 1:A:28:ILE:HA | 1:A:31:LEU:HD11 | 2 | 0.18 | 0.04 | 0.18 |
| (2,328) | 2:B:163:ALA:H | 2:B:162:LEU:HB2 | 2 | 0.18 | 0.0 | 0.18 |
| (2,328) | 2:B:163:ALA:H | 2:B:162:LEU:HB3 | 2 | 0.18 | 0.0 | 0.18 |
| (2,846) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 2 | 0.18 | 0.06 | 0.18 |
| (2,846) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 2 | 0.18 | 0.06 | 0.18 |
| (2,846) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 2 | 0.18 | 0.06 | 0.18 |
| (2,846) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 2 | 0.18 | 0.06 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 2 | 0.18 | 0.0 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 2 | 0.18 | 0.0 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 2 | 0.18 | 0.0 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 2 | 0.18 | 0.0 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,3392) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 2 | 0.18 | 0.0 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD12 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD11 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD13 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:109:LEU:HD13 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD12 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD11 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD13 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD12 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD11 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD13 | 2 | 0.18 | 0.02 | 0.18 |
| (2,3025) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HE2 | 2 | 0.17 | 0.06 | 0.17 |
| (2,3025) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HE3 | 2 | 0.17 | 0.06 | 0.17 |
| (2,3025) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HE2 | 2 | 0.17 | 0.06 | 0.17 |
| (2,3025) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HE3 | 2 | 0.17 | 0.06 | 0.17 |
| (2,3025) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HE2 | 2 | 0.17 | 0.06 | 0.17 |
| (2,3025) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HE3 | 2 | 0.17 | 0.06 | 0.17 |
| (2,677) | 1:A:49:LYS:HB2 | 1:A:49:LYS:HD2 | 2 | 0.17 | 0.01 | 0.17 |
| (2,677) | 1:A:49:LYS:HB3 | 1:A:49:LYS:HD2 | 2 | 0.17 | 0.01 | 0.17 |
| (2,677) | 1:A:49:LYS:HB3 | 1:A:49:LYS:HD3 | 2 | 0.17 | 0.01 | 0.17 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE2 | 2 | 0.16 | 0.04 | 0.16 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE1 | 2 | 0.16 | 0.04 | 0.16 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE3 | 2 | 0.16 | 0.04 | 0.16 |
| (2,2538) | 1:A:58:SER:HB2 | 1:A:55:ASN:HB2 | 2 | 0.16 | 0.01 | 0.16 |
| (2,2538) | 1:A:58:SER:HB2 | 1:A:55:ASN:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,2538) | 1:A:58:SER:HB3 | 1:A:55:ASN:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,2871) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 2 | 0.16 | 0.01 | 0.16 |
| (2,2871) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,498) | 1:A:25:GLU:HG2 | 1:A:48:ALA:HB1 | 2 | 0.16 | 0.02 | 0.16 |
| (2,498) | 1:A:25:GLU:HG2 | 1:A:48:ALA:HB3 | 2 | 0.16 | 0.02 | 0.16 |
| (2,498) | 1:A:25:GLU:HG3 | 1:A:48:ALA:HB1 | 2 | 0.16 | 0.02 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,498) | 1:A:25:GLU:HG3 | 1:A:48:ALA:HB3 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:109:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (2,332) | 2:B:165:VAL:H | 2:B:164:SER:HB2 | 2 | 0.16 | 0.02 | 0.16 |
| (2,332) | 2:B:165:VAL:H | 2:B:164:SER:HB3 | 2 | 0.16 | 0.02 | 0.16 |
| (2,4524) | 2:B:146:LEU:H | 2:B:146:LEU:HG | 2 | 0.16 | 0.01 | 0.16 |
| (2,3528) | 1:A:5:SER:H | 1:A:3:SER:HA | 2 | 0.15 | 0.02 | 0.15 |
| (1,67) | 2:B:113:GLY:N | 2:B:109:LEU:O | 2 | 0.15 | 0.0 | 0.15 |
| (1,68) | 2:B:113:GLY:H | 2:B:109:LEU:O | 2 | 0.15 | 0.0 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG12 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG11 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG13 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG12 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG11 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG13 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG12 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG11 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG13 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG22 | 2 | 0.15 | 0.03 | 0.15 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG23 | 2 | 0.15 | 0.03 | 0.15 |
| (1,25) | 1:A:28:ILE:N | 1:A:24:THR:O | 2 | 0.15 | 0.0 | 0.15 |
| (2,671) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 2 | 0.15 | 0.0 | 0.15 |
| (2,671) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 2 | 0.15 | 0.0 | 0.15 |
| (2,2717) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HD21 | 2 | 0.15 | 0.03 | 0.15 |
| (2,2717) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HD21 | 2 | 0.15 | 0.03 | 0.15 |
| (2,2717) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HD21 | 2 | 0.15 | 0.03 | 0.15 |
| (2,735) | 1:A:59:LEU:HA | 1:A:59:LEU:HD22 | 2 | 0.14 | 0.0 | 0.14 |
| (2,735) | 1:A:59:LEU:HA | 1:A:59:LEU:HD21 | 2 | 0.14 | 0.0 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (2,1758) | 2:B:126:ILE:HA | 2:B:125:LYS:HD2 | 2 | 0.14 | 0.01 | 0.14 |
| (2,1758) | 2:B:126:ILE:HA | 2:B:125:LYS:HD3 | 2 | 0.14 | 0.01 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD23 | 1:A:27:LYS:HE3 | 2 | 0.14 | 0.02 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD12 | 1:A:27:LYS:HE2 | 2 | 0.14 | 0.02 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD12 | 1:A:27:LYS:HE3 | 2 | 0.14 | 0.02 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD11 | 1:A:27:LYS:HE2 | 2 | 0.14 | 0.02 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD11 | 1:A:27:LYS:HE3 | 2 | 0.14 | 0.02 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD22 | 1:A:27:LYS:HE2 | 2 | 0.14 | 0.02 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD22 | 1:A:27:LYS:HE3 | 2 | 0.14 | 0.02 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD21 | 1:A:27:LYS:HE3 | 2 | 0.14 | 0.02 | 0.14 |
| (2,2166) | 1:A:16:LEU:HD23 | 1:A:27:LYS:HE2 | 2 | 0.14 | 0.02 | 0.14 |
| (2,4001) | 2:B:164:SER:H | 2:B:163:ALA:HA | 2 | 0.14 | 0.01 | 0.14 |
| (1,91) | 2:B:144:SER:N | 2:B:140:ASN:O | 2 | 0.13 | 0.01 | 0.13 |
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG12 | 2 | 0.13 | 0.01 | 0.13 |
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG11 | 2 | 0.13 | 0.01 | 0.13 |
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG13 | 2 | 0.13 | 0.01 | 0.13 |
| (2,919) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 2 | 0.13 | 0.0 | 0.13 |
| (2,919) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 2 | 0.13 | 0.0 | 0.13 |
| (2,919) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 2 | 0.13 | 0.0 | 0.13 |
| (2,1162) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 2 | 0.13 | 0.01 | 0.13 |
| (2,1162) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 2 | 0.13 | 0.01 | 0.13 |
| (2,1162) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 2 | 0.13 | 0.01 | 0.13 |
| (2,560) | 1:A:33:LYS:HA | 1:A:33:LYS:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (2,560) | 1:A:33:LYS:HA | 1:A:33:LYS:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,1236) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 2 | 0.12 | 0.01 | 0.12 |
| (2,1236) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG22 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG21 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG23 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB3 | 1:A:4:VAL:HG21 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB3 | 1:A:4:VAL:HG23 | 2 | 0.12 | 0.01 | 0.12 |
| (1,99) | 2:B:155:ILE:N | 2:B:151:ILE:O | 2 | 0.12 | 0.0 | 0.12 |
| (2,1934) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,1934) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,1934) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG22 | 1:A:47:PHE:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG22 | 1:A:9:CYS:H | 2 | 0.12 | 0.0 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:47:PHE:HE1 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:47:PHE:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:9:CYS:H | 2 | 0.12 | 0.0 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG23 | 1:A:47:PHE:HE1 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG23 | 1:A:47:PHE:HE2 | 2 | 0.12 | 0.0 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,3270) | 2:B:165:VAL:HG12 | 2:B:161:LYS:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3270) | 2:B:165:VAL:HG12 | 2:B:161:LYS:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3270) | 2:B:165:VAL:HG11 | 2:B:161:LYS:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3270) | 2:B:165:VAL:HG11 | 2:B:161:LYS:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3270) | 2:B:165:VAL:HG13 | 2:B:161:LYS:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3270) | 2:B:165:VAL:HG23 | 2:B:161:LYS:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (2,3270) | 2:B:165:VAL:HG23 | 2:B:161:LYS:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,73) | 2:B:125:LYS:N | 2:B:121:LYS:O | 2 | 0.12 | 0.0 | 0.12 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (2,337) | 2:B:169:GLY:H | 2:B:168:GLY:HA2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,337) | 2:B:169:GLY:H | 2:B:168:GLY:HA3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,430) | 1:A:15:ILE:HG22 | 2:B:106:SER:HA | 2 | 0.12 | 0.0 | 0.12 |
| (2,430) | 1:A:15:ILE:HG23 | 2:B:106:SER:HA | 2 | 0.12 | 0.0 | 0.12 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG12 | 1:A:7:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE1 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2992) | 2:B:137:ASP:HA | 2:B:140:ASN:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2992) | 2:B:137:ASP:HA | 2:B:140:ASN:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,3011) | 2:B:137:ASP:HB3 | 2:B:138:ARG:HG2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,3011) | 2:B:137:ASP:HB2 | 2:B:138:ARG:HG2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 2 | 0.12 | 0.0 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 2 | 0.12 | 0.0 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 2 | 0.12 | 0.0 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 2 | 0.12 | 0.0 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 2 | 0.12 | 0.0 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |

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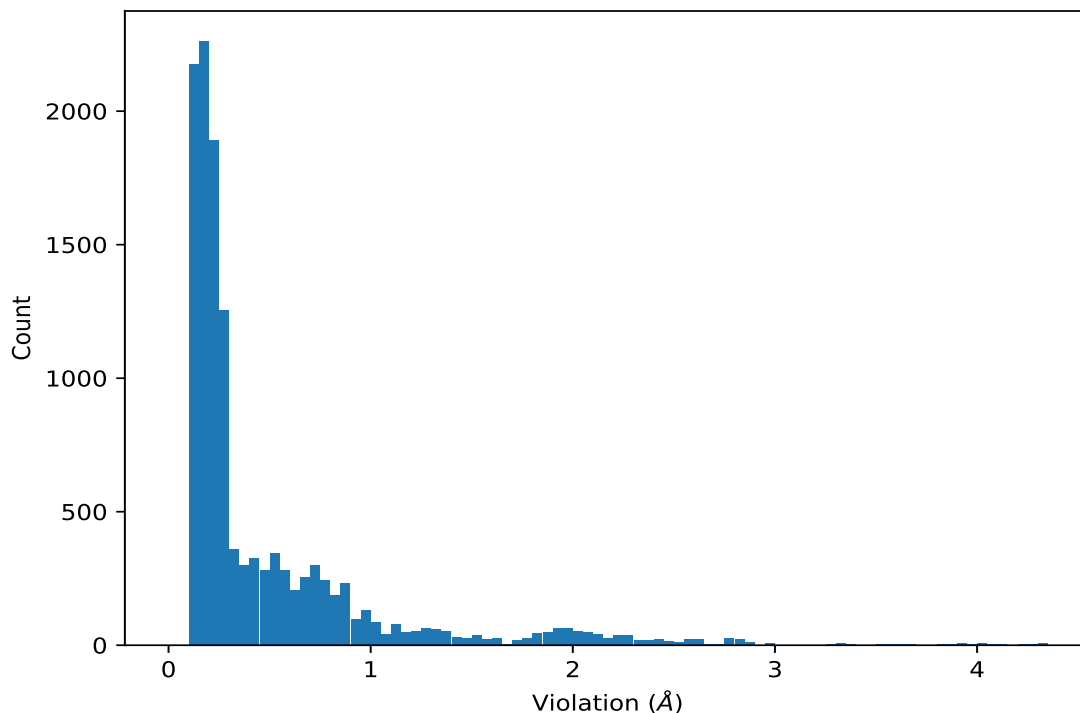
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,3391) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (2,2456) | 1:A:46:LEU:HD22 | 1:A:42:PHE:HZ | 2 | 0.11 | 0.0 | 0.11 |
| (2,2456) | 1:A:46:LEU:HD21 | 1:A:42:PHE:HZ | 2 | 0.11 | 0.0 | 0.11 |
| (2,2456) | 1:A:46:LEU:HD23 | 1:A:42:PHE:HZ | 2 | 0.11 | 0.0 | 0.11 |
| (2,3301) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HA | 2 | 0.11 | 0.0 | 0.11 |
| (2,3301) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HA | 2 | 0.11 | 0.0 | 0.11 |
| (2,3736) | 1:A:58:SER:H | 1:A:55:ASN:HA | 2 | 0.11 | 0.0 | 0.11 |
| (2,3745) | 1:A:61:CYS:H | 1:A:62:ASN:HA | 2 | 0.11 | 0.0 | 0.11 |

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) |
|----------|-----------------|-----------------|----------|---------------|
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 6 | 4.33 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 9 | 4.33 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 8 | 4.32 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 2 | 4.3 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 4 | 4.3 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 5 | 4.3 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 10 | 4.28 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 3 | 4.27 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 7 | 4.24 |
| (2,4060) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 1 | 4.21 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 6 | 4.12 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 9 | 4.12 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 8 | 4.11 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 2 | 4.08 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 4 | 4.08 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 5 | 4.08 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 3 | 4.06 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 10 | 4.06 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 7 | 4.03 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 8 | 4.02 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 10 | 4.02 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 1 | 4.01 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 4 | 4.01 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 7 | 4.0 |
| (2,4402) | 1:A:11:TYR:HE1 | 2:B:112:LEU:HG | 1 | 3.99 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 5 | 3.98 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 8 | 3.93 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 10 | 3.93 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 1 | 3.92 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 4 | 3.92 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 7 | 3.91 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 2 | 3.9 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 3 | 3.9 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 6 | 3.9 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 9 | 3.89 |
| (2,4249) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 9 | 3.89 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 9 | 3.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 5 | 3.89 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 2 | 3.81 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 3 | 3.81 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 6 | 3.81 |
| (2,4016) | 1:A:14:LEU:HG | 1:A:11:TYR:HD2 | 9 | 3.8 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 8 | 3.69 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 8 | 3.69 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 5 | 3.68 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 5 | 3.68 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 2 | 3.64 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 2 | 3.64 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 6 | 3.61 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 6 | 3.61 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 7 | 3.57 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 7 | 3.57 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 4 | 3.55 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 4 | 3.55 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 1 | 3.53 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 1 | 3.53 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 3 | 3.39 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 6 | 3.39 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 3 | 3.39 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 8 | 3.35 |
| (2,4496) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 10 | 3.34 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 7 | 3.34 |
| (2,4096) | 2:B:138:ARG:HD3 | 2:B:103:TYR:HE1 | 10 | 3.34 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 1 | 3.33 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 4 | 3.31 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 10 | 3.3 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 2 | 3.29 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 3 | 3.29 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 5 | 3.25 |
| (2,4401) | 1:A:11:TYR:HE2 | 2:B:159:ILE:HA | 9 | 3.19 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 1 | 2.95 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 1 | 2.95 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 1 | 2.95 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 1 | 2.95 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 1 | 2.95 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 1 | 2.95 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 6 | 2.85 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 6 | 2.85 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 6 | 2.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 7 | 2.85 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 7 | 2.85 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 7 | 2.85 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 6 | 2.85 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 6 | 2.85 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 6 | 2.85 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 7 | 2.85 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 7 | 2.85 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 7 | 2.85 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 1 | 2.83 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 4 | 2.82 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 5 | 2.82 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 2 | 2.82 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 2 | 2.82 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 2 | 2.82 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 2 | 2.82 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 2 | 2.82 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 2 | 2.82 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 3 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 4 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 4 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 4 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 8 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 8 | 2.8 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 8 | 2.8 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 4 | 2.8 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 4 | 2.8 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 4 | 2.8 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 8 | 2.8 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 8 | 2.8 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 8 | 2.8 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 9 | 2.79 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 10 | 2.79 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 10 | 2.79 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 10 | 2.79 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 10 | 2.79 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 10 | 2.79 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 10 | 2.79 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 2 | 2.77 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 3 | 2.76 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 3 | 2.76 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 3 | 2.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 5 | 2.76 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 5 | 2.76 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 5 | 2.76 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 3 | 2.76 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 3 | 2.76 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 3 | 2.76 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 5 | 2.76 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 5 | 2.76 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 5 | 2.76 |
| (2,3505) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 9 | 2.75 |
| (2,3505) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 9 | 2.75 |
| (2,3505) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 9 | 2.75 |
| (2,1215) | 2:B:159:ILE:HG22 | 1:A:11:TYR:HE2 | 9 | 2.75 |
| (2,1215) | 2:B:159:ILE:HG21 | 1:A:11:TYR:HE2 | 9 | 2.75 |
| (2,1215) | 2:B:159:ILE:HG23 | 1:A:11:TYR:HE2 | 9 | 2.75 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 10 | 2.73 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 6 | 2.7 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 7 | 2.7 |
| (2,4078) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 8 | 2.7 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 9 | 2.66 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 9 | 2.66 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 9 | 2.64 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 9 | 2.64 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 10 | 2.63 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 10 | 2.63 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 3 | 2.62 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 3 | 2.62 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 8 | 2.62 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 8 | 2.62 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 5 | 2.61 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 5 | 2.61 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 10 | 2.61 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 10 | 2.61 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 8 | 2.6 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 8 | 2.6 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 8 | 2.6 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 4 | 2.6 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 4 | 2.6 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 3 | 2.6 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 3 | 2.6 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 8 | 2.6 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 8 | 2.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 2 | 2.59 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 2 | 2.59 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 5 | 2.59 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 5 | 2.59 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 4 | 2.58 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 4 | 2.58 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 2 | 2.57 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 2 | 2.57 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 3 | 2.56 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 3 | 2.56 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 3 | 2.56 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 6 | 2.56 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 6 | 2.56 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 6 | 2.56 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 7 | 2.56 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 7 | 2.56 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 5 | 2.55 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 5 | 2.55 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 5 | 2.55 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 6 | 2.55 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 6 | 2.55 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 1 | 2.55 |
| (2,695) | 1:A:51:LEU:HD12 | 1:A:48:ALA:HA | 6 | 2.54 |
| (2,695) | 1:A:51:LEU:HD11 | 1:A:48:ALA:HA | 6 | 2.54 |
| (2,695) | 1:A:51:LEU:HD13 | 1:A:48:ALA:HA | 6 | 2.54 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 4 | 2.54 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 5 | 2.54 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 7 | 2.54 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 7 | 2.54 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 6 | 2.53 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 6 | 2.53 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 3 | 2.52 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 9 | 2.51 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 3 | 2.49 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 3 | 2.49 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 3 | 2.49 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 3 | 2.49 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 2 | 2.49 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 9 | 2.48 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 9 | 2.48 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 9 | 2.48 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 2 | 2.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 2 | 2.47 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 2 | 2.47 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 7 | 2.47 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 7 | 2.47 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 7 | 2.47 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 10 | 2.45 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 1 | 2.44 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 1 | 2.44 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 1 | 2.44 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 10 | 2.44 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 10 | 2.44 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 10 | 2.44 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 7 | 2.43 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 7 | 2.43 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 7 | 2.43 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 7 | 2.43 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 6 | 2.42 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 7 | 2.42 |
| (2,4427) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 8 | 2.42 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 4 | 2.41 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 4 | 2.41 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 4 | 2.41 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 4 | 2.41 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 2 | 2.4 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 2 | 2.4 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 2 | 2.4 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 2 | 2.4 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 1 | 2.38 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 1 | 2.38 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 1 | 2.38 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 1 | 2.38 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 5 | 2.37 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 5 | 2.37 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 5 | 2.37 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 5 | 2.37 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 1 | 2.37 |
| (2,759) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 1 | 2.37 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 10 | 2.35 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 10 | 2.35 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 10 | 2.35 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 10 | 2.35 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 10 | 2.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 10 | 2.35 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 1 | 2.35 |
| (2,2599) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 1 | 2.35 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 1 | 2.34 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 4 | 2.34 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 5 | 2.34 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 3 | 2.34 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 3 | 2.34 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 3 | 2.34 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 3 | 2.34 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 3 | 2.33 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 3 | 2.33 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 3 | 2.33 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 3 | 2.33 |
| (2,799) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 4 | 2.32 |
| (2,799) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 4 | 2.32 |
| (2,799) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 4 | 2.32 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 3 | 2.31 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 10 | 2.3 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 10 | 2.3 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 10 | 2.3 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 2.3 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 9 | 2.3 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 9 | 2.28 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 9 | 2.28 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 9 | 2.28 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 9 | 2.28 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 2 | 2.28 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 7 | 2.28 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 7 | 2.28 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 7 | 2.28 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 7 | 2.28 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 7 | 2.27 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 7 | 2.27 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 7 | 2.27 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 7 | 2.27 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 6 | 2.27 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 6 | 2.27 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 6 | 2.27 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 6 | 2.26 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 6 | 2.26 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 6 | 2.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 6 | 2.26 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 6 | 2.26 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 6 | 2.26 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 4 | 2.26 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 4 | 2.26 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 4 | 2.26 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 4 | 2.26 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 6 | 2.26 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 6 | 2.26 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 2 | 2.25 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 2 | 2.25 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 2 | 2.25 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 2 | 2.25 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 4 | 2.25 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 4 | 2.25 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 4 | 2.25 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 4 | 2.25 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 10 | 2.24 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 2 | 2.24 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 2 | 2.24 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 2 | 2.24 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 2 | 2.24 |
| (2,869) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 8 | 2.23 |
| (2,869) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 8 | 2.23 |
| (2,869) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 8 | 2.23 |
| (2,869) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 8 | 2.23 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 4 | 2.23 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 4 | 2.23 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 1 | 2.23 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 1 | 2.23 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 1 | 2.23 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 1 | 2.23 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 4 | 2.23 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 4 | 2.23 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 6 | 2.22 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 7 | 2.22 |
| (2,4573) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 8 | 2.22 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 5 | 2.22 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 5 | 2.22 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 5 | 2.22 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 5 | 2.22 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 1 | 2.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 1 | 2.22 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 1 | 2.22 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 1 | 2.22 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 5 | 2.21 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 5 | 2.21 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 5 | 2.21 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 5 | 2.21 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 5 | 2.2 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 5 | 2.2 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 5 | 2.2 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 5 | 2.2 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 3 | 2.16 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 3 | 2.16 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 8 | 2.16 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 8 | 2.16 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 8 | 2.16 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 9 | 2.16 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 9 | 2.16 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 3 | 2.16 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 3 | 2.16 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 10 | 2.15 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 10 | 2.15 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 10 | 2.15 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 7 | 2.15 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 7 | 2.15 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 2.15 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 10 | 2.15 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 10 | 2.15 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 10 | 2.15 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 10 | 2.15 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 10 | 2.15 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 10 | 2.15 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 7 | 2.15 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 7 | 2.15 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 4 | 2.15 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 4 | 2.15 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 4 | 2.15 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 6 | 2.14 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 6 | 2.14 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 6 | 2.14 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 6 | 2.14 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 6 | 2.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 6 | 2.14 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 10 | 2.14 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 10 | 2.14 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 2.14 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 10 | 2.14 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 10 | 2.13 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 10 | 2.13 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 9 | 2.13 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 9 | 2.13 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 9 | 2.13 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 9 | 2.13 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 10 | 2.13 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 10 | 2.13 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 3 | 2.12 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 3 | 2.12 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 3 | 2.12 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 6 | 2.12 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 6 | 2.12 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 6 | 2.12 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 9 | 2.12 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 9 | 2.12 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 9 | 2.12 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 9 | 2.12 |
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 6 | 2.11 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 6 | 2.11 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 6 | 2.11 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 6 | 2.11 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 5 | 2.11 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 5 | 2.11 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 5 | 2.11 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 5 | 2.1 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 5 | 2.1 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 6 | 2.1 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 6 | 2.1 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 6 | 2.1 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 6 | 2.1 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 10 | 2.09 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 10 | 2.09 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 10 | 2.09 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 5 | 2.08 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 5 | 2.08 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 5 | 2.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,3449) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 8 | 2.08 |
| (2,3449) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 8 | 2.08 |
| (2,3449) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 8 | 2.08 |
| (2,3449) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 8 | 2.08 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 5 | 2.08 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 5 | 2.08 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 5 | 2.08 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 1 | 2.07 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 1 | 2.07 |
| (2,2740) | 2:B:112:LEU:HD11 | 1:A:11:TYR:HE1 | 8 | 2.07 |
| (2,2740) | 2:B:112:LEU:HD13 | 1:A:11:TYR:HE1 | 8 | 2.07 |
| (2,2740) | 2:B:112:LEU:HD22 | 1:A:11:TYR:HE1 | 8 | 2.07 |
| (2,2740) | 2:B:112:LEU:HD12 | 1:A:11:TYR:HE1 | 8 | 2.07 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 4 | 2.06 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 4 | 2.06 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 4 | 2.06 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 8 | 2.06 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 8 | 2.06 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 8 | 2.06 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 2 | 2.05 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 2 | 2.05 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 2 | 2.05 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 2 | 2.05 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 2 | 2.05 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 8 | 2.05 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 8 | 2.05 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 6 | 2.05 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 6 | 2.05 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 6 | 2.05 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 6 | 2.05 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 6 | 2.05 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 6 | 2.05 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 2 | 2.05 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 2 | 2.05 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 2 | 2.05 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 2 | 2.05 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 2 | 2.05 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 8 | 2.05 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 8 | 2.05 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 6 | 2.05 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 6 | 2.05 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 6 | 2.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 5 | 2.04 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 5 | 2.04 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 5 | 2.04 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 9 | 2.04 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 9 | 2.04 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 9 | 2.04 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 9 | 2.04 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 9 | 2.04 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 5 | 2.04 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 5 | 2.04 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 5 | 2.04 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 9 | 2.04 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 9 | 2.04 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 2 | 2.03 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 2 | 2.03 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 2 | 2.03 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 7 | 2.03 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 7 | 2.03 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 7 | 2.03 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 8 | 2.03 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 8 | 2.03 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 3 | 2.02 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 3 | 2.02 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 6 | 2.02 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 6 | 2.02 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 6 | 2.02 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 2 | 2.02 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 2 | 2.02 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 2 | 2.02 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 4 | 2.01 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 4 | 2.01 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 7 | 2.01 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 7 | 2.01 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 3 | 2.01 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 3 | 2.01 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 3 | 2.01 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 1 | 2.0 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 1 | 2.0 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 1 | 2.0 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 10 | 2.0 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 10 | 2.0 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 10 | 2.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 10 | 2.0 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 10 | 2.0 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 10 | 2.0 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 5 | 2.0 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 5 | 2.0 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 5 | 2.0 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 6 | 2.0 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 6 | 2.0 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 6 | 2.0 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 6 | 2.0 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 6 | 2.0 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 6 | 2.0 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 7 | 1.99 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 7 | 1.99 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 7 | 1.99 |
| (2,396) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 1 | 1.99 |
| (2,396) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 1 | 1.99 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 2 | 1.99 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 2 | 1.99 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 6 | 1.99 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 6 | 1.99 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 7 | 1.99 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 7 | 1.99 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 7 | 1.99 |
| (2,2101) | 1:A:10:ILE:HG21 | 1:A:11:TYR:HD2 | 1 | 1.99 |
| (2,2101) | 1:A:10:ILE:HG22 | 1:A:11:TYR:HD2 | 1 | 1.99 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 1 | 1.99 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 3 | 1.99 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 3 | 1.99 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 3 | 1.99 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 8 | 1.99 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 8 | 1.99 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 8 | 1.99 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 1 | 1.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 1 | 1.98 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 1 | 1.98 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 6 | 1.98 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 6 | 1.98 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 6 | 1.98 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 1 | 1.98 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 1 | 1.98 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 1 | 1.98 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 6 | 1.98 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 6 | 1.98 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 6 | 1.98 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 4 | 1.96 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 4 | 1.96 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 4 | 1.96 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 9 | 1.96 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 9 | 1.96 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 4 | 1.96 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 4 | 1.96 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 4 | 1.96 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 4 | 1.96 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 3 | 1.95 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 3 | 1.95 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 3 | 1.95 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 3 | 1.95 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 3 | 1.95 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 3 | 1.95 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 7 | 1.94 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 7 | 1.94 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 7 | 1.94 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 7 | 1.94 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 7 | 1.94 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 7 | 1.94 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 7 | 1.94 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 7 | 1.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 7 | 1.94 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 10 | 1.93 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 10 | 1.93 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 2 | 1.93 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 2 | 1.93 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 2 | 1.93 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 9 | 1.93 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 9 | 1.93 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 9 | 1.93 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 8 | 1.92 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 8 | 1.92 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 8 | 1.92 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 2 | 1.92 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 2 | 1.92 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 2 | 1.92 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 3 | 1.92 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 3 | 1.92 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 8 | 1.92 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 8 | 1.92 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 8 | 1.92 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 8 | 1.92 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 8 | 1.92 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 2 | 1.92 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 2 | 1.92 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 2 | 1.92 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 2 | 1.92 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 2 | 1.92 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 2 | 1.92 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 7 | 1.92 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 7 | 1.92 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 7 | 1.92 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 10 | 1.92 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 5 | 1.91 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 5 | 1.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 4 | 1.9 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 4 | 1.9 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 3 | 1.9 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 3 | 1.9 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 3 | 1.9 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 8 | 1.9 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 8 | 1.9 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 8 | 1.9 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 1 | 1.9 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 1 | 1.9 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 1 | 1.9 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 10 | 1.9 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 10 | 1.9 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 10 | 1.9 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 2 | 1.89 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 2 | 1.89 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 1 | 1.89 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 1 | 1.89 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 1 | 1.89 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 3 | 1.88 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 3 | 1.88 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 3 | 1.88 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 7 | 1.88 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 7 | 1.88 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 7 | 1.88 |
| (2,3423) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 4 | 1.88 |
| (2,3423) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 4 | 1.88 |
| (2,3423) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 4 | 1.88 |
| (2,3008) | 2:B:138:ARG:HG2 | 2:B:103:TYR:HD1 | 10 | 1.88 |
| (2,3008) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HD1 | 10 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 3 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 3 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 3 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 7 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 7 | 1.88 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 7 | 1.88 |
| (2,978) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 9 | 1.87 |
| (2,978) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 9 | 1.87 |
| (2,978) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 9 | 1.87 |
| (2,2909) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HE2 | 9 | 1.87 |
| (2,2909) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HE2 | 9 | 1.87 |
| (2,2909) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HE2 | 9 | 1.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 1 | 1.86 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 1 | 1.86 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 1 | 1.86 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 7 | 1.86 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 7 | 1.86 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 1 | 1.86 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 1 | 1.86 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 1 | 1.86 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 8 | 1.85 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 8 | 1.85 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 8 | 1.85 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 6 | 1.85 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 6 | 1.85 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 4 | 1.85 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 8 | 1.85 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 8 | 1.85 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 8 | 1.85 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 5 | 1.85 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 5 | 1.85 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 5 | 1.85 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 6 | 1.84 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 6 | 1.84 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 6 | 1.84 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 7 | 1.84 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 7 | 1.84 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 7 | 1.84 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 8 | 1.83 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 4 | 1.82 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 4 | 1.82 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 4 | 1.82 |
| (2,977) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 9 | 1.82 |
| (2,977) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 9 | 1.82 |
| (2,977) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 9 | 1.82 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 3 | 1.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 4 | 1.82 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 4 | 1.82 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 4 | 1.82 |
| (2,2905) | 2:B:127:LEU:HD22 | 2:B:103:TYR:HD2 | 9 | 1.82 |
| (2,2905) | 2:B:127:LEU:HD21 | 2:B:103:TYR:HD2 | 9 | 1.82 |
| (2,2905) | 2:B:127:LEU:HD23 | 2:B:103:TYR:HD2 | 9 | 1.82 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 9 | 1.82 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 1 | 1.8 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 5 | 1.8 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 8 | 1.8 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 1 | 1.8 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 1 | 1.8 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 1 | 1.8 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 4 | 1.79 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 7 | 1.79 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 6 | 1.78 |
| (2,2656) | 2:B:105:ALA:HB2 | 1:A:11:TYR:HD2 | 4 | 1.78 |
| (2,2656) | 2:B:105:ALA:HB1 | 1:A:11:TYR:HD2 | 4 | 1.78 |
| (2,2656) | 2:B:105:ALA:HB3 | 1:A:11:TYR:HD2 | 4 | 1.78 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 2 | 1.76 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 10 | 1.76 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 5 | 1.76 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 5 | 1.76 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 5 | 1.76 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 2 | 1.76 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 1 | 1.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 6 | 1.75 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 6 | 1.75 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 6 | 1.75 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 7 | 1.75 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 7 | 1.75 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 7 | 1.75 |
| (2,3826) | 2:B:120:ALA:H | 2:B:121:LYS:HB3 | 9 | 1.74 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 3 | 1.72 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 3 | 1.71 |
| (2,3336) | 1:A:15:ILE:HD12 | 2:B:109:LEU:HD22 | 4 | 1.7 |
| (2,3336) | 1:A:15:ILE:HD12 | 2:B:109:LEU:HD21 | 4 | 1.7 |
| (2,3336) | 1:A:15:ILE:HD11 | 2:B:109:LEU:HD22 | 4 | 1.7 |
| (2,3336) | 1:A:15:ILE:HD11 | 2:B:109:LEU:HD21 | 4 | 1.7 |
| (2,3336) | 1:A:15:ILE:HD11 | 2:B:109:LEU:HD23 | 4 | 1.7 |
| (2,3336) | 1:A:15:ILE:HD13 | 2:B:109:LEU:HD22 | 4 | 1.7 |
| (2,3336) | 1:A:15:ILE:HD13 | 2:B:109:LEU:HD21 | 4 | 1.7 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 9 | 1.68 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 1 | 1.67 |
| (2,762) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 1 | 1.67 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 10 | 1.66 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 5 | 1.64 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 9 | 1.64 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 9 | 1.64 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 8 | 1.63 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 2 | 1.61 |
| (2,3499) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 5 | 1.61 |
| (2,3499) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 5 | 1.61 |
| (2,3499) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 5 | 1.61 |
| (2,3223) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 5 | 1.61 |
| (2,3223) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 5 | 1.61 |
| (2,3223) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 5 | 1.61 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 10 | 1.61 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 10 | 1.61 |
| (2,1209) | 2:B:159:ILE:HD12 | 1:A:11:TYR:HE2 | 5 | 1.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1209) | 2:B:159:ILE:HD11 | 1:A:11:TYR:HE2 | 5 | 1.61 |
| (2,1209) | 2:B:159:ILE:HD13 | 1:A:11:TYR:HE2 | 5 | 1.61 |
| (2,1027) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 9 | 1.61 |
| (2,1027) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 9 | 1.61 |
| (2,1027) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 9 | 1.61 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 9 | 1.6 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 9 | 1.6 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 3 | 1.6 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 3 | 1.6 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 5 | 1.6 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 5 | 1.6 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 8 | 1.6 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 8 | 1.6 |
| (2,842) | 2:B:109:LEU:HD21 | 1:A:12:SER:HA | 4 | 1.59 |
| (2,842) | 2:B:109:LEU:HD23 | 1:A:12:SER:HA | 4 | 1.59 |
| (2,842) | 2:B:109:LEU:HD22 | 1:A:12:SER:HA | 4 | 1.59 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 6 | 1.59 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 10 | 1.59 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 10 | 1.59 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 4 | 1.59 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 4 | 1.59 |
| (2,2709) | 2:B:109:LEU:HD22 | 1:A:12:SER:HA | 4 | 1.58 |
| (2,2709) | 2:B:109:LEU:HD21 | 1:A:12:SER:HA | 4 | 1.58 |
| (2,2709) | 2:B:109:LEU:HD23 | 1:A:12:SER:HA | 4 | 1.58 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 8 | 1.58 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 8 | 1.58 |
| (2,4011) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 7 | 1.57 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 2 | 1.57 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 2 | 1.57 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 2 | 1.56 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 2 | 1.56 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 1 | 1.55 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 7 | 1.55 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 7 | 1.55 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 7 | 1.54 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 4 | 1.53 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 5 | 1.53 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 3 | 1.53 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 3 | 1.53 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 4 | 1.53 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 4 | 1.53 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 7 | 1.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 7 | 1.53 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 6 | 1.53 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 6 | 1.53 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 10 | 1.53 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 10 | 1.53 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 3 | 1.53 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 3 | 1.53 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 3 | 1.53 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 3 | 1.53 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 6 | 1.52 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 8 | 1.52 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 10 | 1.52 |
| (2,2975) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HE2 | 9 | 1.52 |
| (2,2975) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HE2 | 9 | 1.52 |
| (2,2975) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HE2 | 9 | 1.52 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 5 | 1.52 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 5 | 1.52 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 10 | 1.52 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 10 | 1.52 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 10 | 1.52 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 2 | 1.51 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 9 | 1.51 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 5 | 1.51 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 5 | 1.51 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 6 | 1.51 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 6 | 1.51 |
| (2,4241) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 3 | 1.5 |
| (2,3269) | 2:B:165:VAL:H | 2:B:165:VAL:HG22 | 7 | 1.5 |
| (2,3269) | 2:B:165:VAL:H | 2:B:165:VAL:HG21 | 7 | 1.5 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 5 | 1.49 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 6 | 1.48 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 6 | 1.48 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 9 | 1.48 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 9 | 1.48 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 7 | 1.48 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 7 | 1.48 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 7 | 1.48 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 7 | 1.48 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 8 | 1.47 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 8 | 1.47 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 8 | 1.47 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 8 | 1.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 10 | 1.47 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 10 | 1.47 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 4 | 1.47 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 4 | 1.47 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 3 | 1.46 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 3 | 1.46 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 3 | 1.46 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 3 | 1.46 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 10 | 1.45 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 10 | 1.45 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 10 | 1.45 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 2 | 1.45 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 2 | 1.45 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 4 | 1.44 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 4 | 1.44 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 4 | 1.44 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 4 | 1.44 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 1 | 1.44 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB3 | 1 | 1.44 |
| (2,2622) | 1:A:11:TYR:HD1 | 1:A:7:LEU:HB2 | 1 | 1.44 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 4 | 1.44 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 4 | 1.44 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 4 | 1.44 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 4 | 1.43 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 5 | 1.43 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 8 | 1.43 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 8 | 1.43 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 8 | 1.43 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 8 | 1.43 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 10 | 1.42 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 10 | 1.42 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 10 | 1.42 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 10 | 1.42 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 1 | 1.42 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 7 | 1.42 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 7 | 1.42 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 3 | 1.41 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 2 | 1.4 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 9 | 1.4 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 8 | 1.4 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 8 | 1.4 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 8 | 1.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 1 | 1.4 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 1 | 1.4 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 6 | 1.39 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 1 | 1.39 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 2 | 1.38 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 7 | 1.38 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 9 | 1.37 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 9 | 1.37 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 9 | 1.37 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 4 | 1.37 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 5 | 1.37 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 4 | 1.37 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 4 | 1.37 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 4 | 1.37 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 2 | 1.37 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 2 | 1.37 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 2 | 1.37 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 2 | 1.37 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 6 | 1.36 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 8 | 1.36 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 10 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 5 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 5 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 5 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 5 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 5 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 5 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 7 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 7 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 7 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 7 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 7 | 1.36 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 7 | 1.36 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB2 | 1 | 1.36 |
| (2,2598) | 1:A:11:TYR:HE1 | 1:A:7:LEU:HB3 | 1 | 1.36 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 6 | 1.36 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 6 | 1.36 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 6 | 1.36 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 6 | 1.36 |
| (2,831) | 2:B:109:LEU:HA | 2:B:109:LEU:HD12 | 4 | 1.35 |
| (2,831) | 2:B:109:LEU:HA | 2:B:109:LEU:HD13 | 4 | 1.35 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 2 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 9 | 1.35 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 8 | 1.35 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 8 | 1.35 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 8 | 1.35 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 8 | 1.35 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 8 | 1.35 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 8 | 1.35 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 5 | 1.35 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 5 | 1.35 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 5 | 1.35 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 5 | 1.35 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 5 | 1.35 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 5 | 1.35 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 5 | 1.35 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 10 | 1.34 |
| (2,4013) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 3 | 1.34 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 10 | 1.34 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 10 | 1.34 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 10 | 1.34 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 10 | 1.34 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 10 | 1.34 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 10 | 1.34 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 1 | 1.34 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 1 | 1.34 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 1 | 1.34 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 5 | 1.34 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 5 | 1.34 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 5 | 1.34 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 9 | 1.33 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 9 | 1.33 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 9 | 1.33 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 9 | 1.33 |
| (2,2706) | 1:A:8:ALA:HA | 2:B:109:LEU:HD12 | 4 | 1.33 |
| (2,2706) | 1:A:8:ALA:HA | 2:B:109:LEU:HD13 | 4 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 4 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 4 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 4 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 4 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 4 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 4 | 1.33 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 3 | 1.33 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 3 | 1.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 8 | 1.33 |
| (2,2187) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 8 | 1.33 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 2 | 1.33 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 2 | 1.33 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 2 | 1.33 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 9 | 1.33 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 9 | 1.33 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 9 | 1.33 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 2 | 1.32 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 2 | 1.32 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 2 | 1.32 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 2 | 1.32 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 2 | 1.32 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 2 | 1.32 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 6 | 1.31 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 7 | 1.31 |
| (2,4411) | 1:A:11:TYR:HD1 | 2:B:109:LEU:HA | 8 | 1.31 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 1 | 1.31 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 1 | 1.31 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 1 | 1.31 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 1 | 1.31 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 1 | 1.31 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 1 | 1.31 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 7 | 1.3 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 3 | 1.3 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 3 | 1.3 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 3 | 1.3 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 3 | 1.3 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 2 | 1.3 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 2 | 1.3 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 2 | 1.3 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 6 | 1.29 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 6 | 1.29 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 4 | 1.29 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 9 | 1.29 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 9 | 1.29 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 9 | 1.29 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 1 | 1.28 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 1 | 1.28 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 1 | 1.28 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 5 | 1.28 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 5 | 1.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 5 | 1.28 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 5 | 1.28 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 5 | 1.28 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 5 | 1.28 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 6 | 1.28 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 6 | 1.28 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 6 | 1.28 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 6 | 1.28 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 6 | 1.28 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 6 | 1.28 |
| (2,1060) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HD2 | 5 | 1.28 |
| (2,1060) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HD2 | 5 | 1.28 |
| (2,1060) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HD2 | 5 | 1.28 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 10 | 1.27 |
| (2,1391) | 1:A:24:THR:HG21 | 1:A:27:LYS:HE3 | 2 | 1.27 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE2 | 2 | 1.27 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE3 | 2 | 1.27 |
| (2,1391) | 1:A:24:THR:HG23 | 1:A:27:LYS:HE3 | 2 | 1.27 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 5 | 1.26 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 5 | 1.26 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 2 | 1.26 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 2 | 1.26 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 2 | 1.26 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 9 | 1.26 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 9 | 1.26 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 9 | 1.26 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 3 | 1.26 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 3 | 1.26 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 3 | 1.26 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 3 | 1.26 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 3 | 1.26 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 3 | 1.26 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 4 | 1.25 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 7 | 1.25 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 7 | 1.25 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 7 | 1.25 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 7 | 1.25 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 7 | 1.25 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 7 | 1.25 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 7 | 1.25 |
| (2,2695) | 2:B:109:LEU:HA | 2:B:109:LEU:HD12 | 4 | 1.25 |
| (2,2695) | 2:B:109:LEU:HA | 2:B:109:LEU:HD13 | 4 | 1.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 9 | 1.25 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 9 | 1.25 |
| (2,2623) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 9 | 1.25 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 9 | 1.25 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 9 | 1.25 |
| (2,2623) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 9 | 1.25 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 10 | 1.25 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 10 | 1.25 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 6 | 1.25 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 6 | 1.25 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 6 | 1.25 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 2 | 1.24 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 2 | 1.24 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 2 | 1.24 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 7 | 1.24 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 7 | 1.24 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 7 | 1.24 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 1 | 1.24 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 1 | 1.24 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 1 | 1.24 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 1 | 1.24 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 8 | 1.23 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 10 | 1.23 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 9 | 1.23 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 9 | 1.23 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 9 | 1.23 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 10 | 1.23 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 10 | 1.23 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 4 | 1.23 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 4 | 1.23 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 4 | 1.23 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 4 | 1.23 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 3 | 1.22 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 3 | 1.22 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 3 | 1.22 |
| (2,4572) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HA | 3 | 1.21 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 5 | 1.21 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 1 | 1.21 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 4 | 1.2 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 4 | 1.2 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 4 | 1.2 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 8 | 1.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 8 | 1.2 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 2 | 1.2 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 4 | 1.2 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 10 | 1.2 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 8 | 1.2 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 8 | 1.2 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 8 | 1.2 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 8 | 1.2 |
| (2,1242) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 1.2 |
| (2,1242) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 1.2 |
| (2,1242) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 1.2 |
| (2,1242) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 1.2 |
| (2,1242) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 1.2 |
| (2,1242) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 1.2 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 8 | 1.2 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 8 | 1.2 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 8 | 1.2 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 10 | 1.2 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 10 | 1.2 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 10 | 1.2 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 10 | 1.2 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 1 | 1.19 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 3 | 1.19 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 6 | 1.19 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 6 | 1.19 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 6 | 1.19 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 4 | 1.19 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 4 | 1.19 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 4 | 1.19 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 9 | 1.19 |
| (2,1057) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 9 | 1.19 |
| (2,1057) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 9 | 1.19 |
| (2,1057) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 9 | 1.19 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 3 | 1.18 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 6 | 1.18 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 8 | 1.18 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 5 | 1.18 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 7 | 1.18 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 7 | 1.18 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 7 | 1.18 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 10 | 1.18 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 10 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 1 | 1.18 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 1 | 1.18 |
| (2,1182) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 10 | 1.18 |
| (2,1182) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 10 | 1.18 |
| (2,1182) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 10 | 1.18 |
| (2,836) | 1:A:8:ALA:HA | 2:B:109:LEU:HD12 | 4 | 1.17 |
| (2,836) | 1:A:8:ALA:HA | 2:B:109:LEU:HD13 | 4 | 1.17 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 3 | 1.17 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 2 | 1.17 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 4 | 1.17 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 3 | 1.17 |
| (2,331) | 2:B:165:VAL:H | 2:B:165:VAL:HG22 | 7 | 1.17 |
| (2,331) | 2:B:165:VAL:H | 2:B:165:VAL:HG21 | 7 | 1.17 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 1 | 1.16 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 3 | 1.16 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 3 | 1.16 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 3 | 1.16 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 5 | 1.16 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 5 | 1.16 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 6 | 1.16 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 6 | 1.16 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 6 | 1.15 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 9 | 1.15 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 3 | 1.15 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 6 | 1.15 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 8 | 1.15 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 6 | 1.15 |
| (2,832) | 2:B:109:LEU:HA | 2:B:109:LEU:HD13 | 4 | 1.14 |
| (2,832) | 2:B:109:LEU:HA | 2:B:109:LEU:HD12 | 4 | 1.14 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 7 | 1.14 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 7 | 1.14 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 8 | 1.14 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 8 | 1.14 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 8 | 1.14 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 2 | 1.14 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 2 | 1.14 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 2 | 1.14 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 2 | 1.14 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 8 | 1.14 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 8 | 1.14 |
| (2,951) | 2:B:125:LYS:HD2 | 2:B:129:SER:HB3 | 4 | 1.13 |
| (2,951) | 2:B:125:LYS:HD3 | 2:B:129:SER:HB3 | 4 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 1 | 1.13 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 1 | 1.13 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 4 | 1.13 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 4 | 1.13 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 4 | 1.13 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 6 | 1.13 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 6 | 1.13 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 6 | 1.13 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 6 | 1.13 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 9 | 1.13 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 9 | 1.13 |
| (2,1243) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 1.13 |
| (2,1243) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 1.13 |
| (2,1243) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 1.13 |
| (2,1243) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 1.13 |
| (2,1243) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 1.13 |
| (2,1243) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 1.13 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 10 | 1.12 |
| (2,3274) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 1.12 |
| (2,3274) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 1.12 |
| (2,3274) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 1.12 |
| (2,3274) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 1.12 |
| (2,3274) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 1.12 |
| (2,3274) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 1.12 |
| (2,3183) | 2:B:155:ILE:HG22 | 2:B:159:ILE:HG12 | 10 | 1.12 |
| (2,3183) | 2:B:155:ILE:HG21 | 2:B:159:ILE:HG12 | 10 | 1.12 |
| (2,3183) | 2:B:155:ILE:HG23 | 2:B:159:ILE:HG12 | 10 | 1.12 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 5 | 1.12 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 5 | 1.12 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 5 | 1.12 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 5 | 1.12 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 4 | 1.12 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 4 | 1.12 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 7 | 1.11 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 7 | 1.11 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 5 | 1.11 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 9 | 1.11 |
| (2,3386) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD11 | 4 | 1.11 |
| (2,3386) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD13 | 4 | 1.11 |
| (2,3386) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD12 | 4 | 1.11 |
| (2,3386) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD11 | 4 | 1.11 |
| (2,3386) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD13 | 4 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3386) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD11 | 4 | 1.11 |
| (2,3386) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD13 | 4 | 1.11 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 2 | 1.11 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 2 | 1.11 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 4 | 1.11 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 4 | 1.11 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 2 | 1.1 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 2 | 1.1 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 4 | 1.1 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 8 | 1.1 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 8 | 1.1 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 4 | 1.1 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 8 | 1.1 |
| (2,3272) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 1.1 |
| (2,3272) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 1.1 |
| (2,3272) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 1.1 |
| (2,3272) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 1.1 |
| (2,3272) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 1.1 |
| (2,3272) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 1.1 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 2 | 1.1 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 2 | 1.1 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 3 | 1.1 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 3 | 1.1 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 2 | 1.09 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 1 | 1.09 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 2 | 1.09 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 6 | 1.09 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 6 | 1.09 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 2 | 1.08 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 5 | 1.08 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 10 | 1.08 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 10 | 1.08 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 6 | 1.07 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 6 | 1.07 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 6 | 1.07 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 6 | 1.07 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 7 | 1.07 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 7 | 1.07 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 6 | 1.07 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 6 | 1.07 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 3 | 1.06 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 3 | 1.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 3 | 1.06 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 4 | 1.06 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 6 | 1.06 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 4 | 1.06 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 4 | 1.06 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 4 | 1.06 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 9 | 1.06 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 9 | 1.06 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 9 | 1.05 |
| (2,374) | 1:A:8:ALA:HA | 2:B:109:LEU:HD12 | 4 | 1.05 |
| (2,374) | 1:A:8:ALA:HA | 2:B:109:LEU:HD13 | 4 | 1.05 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 6 | 1.05 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 6 | 1.05 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 2 | 1.05 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 2 | 1.05 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 2 | 1.05 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 1 | 1.05 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 1 | 1.05 |
| (2,1936) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 10 | 1.05 |
| (2,1936) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 10 | 1.05 |
| (2,1936) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 10 | 1.05 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 10 | 1.05 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 10 | 1.05 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 3 | 1.04 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 3 | 1.04 |
| (2,4230) | 1:A:8:ALA:HA | 1:A:11:TYR:HD1 | 7 | 1.04 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 5 | 1.04 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 5 | 1.04 |
| (2,969) | 2:B:127:LEU:HB2 | 2:B:124:LYS:HD2 | 5 | 1.03 |
| (2,969) | 2:B:127:LEU:HB3 | 2:B:124:LYS:HD2 | 5 | 1.03 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 5 | 1.03 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 5 | 1.03 |
| (2,3435) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD12 | 4 | 1.03 |
| (2,3435) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD11 | 4 | 1.03 |
| (2,3435) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD11 | 4 | 1.03 |
| (2,3435) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD11 | 4 | 1.03 |
| (2,3435) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD13 | 4 | 1.03 |
| (2,3435) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD13 | 4 | 1.03 |
| (2,3435) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD13 | 4 | 1.03 |
| (2,3435) | 1:A:15:ILE:HD12 | 2:B:109:LEU:HD22 | 4 | 1.03 |
| (2,3435) | 1:A:15:ILE:HD11 | 2:B:109:LEU:HD22 | 4 | 1.03 |
| (2,3435) | 1:A:15:ILE:HD13 | 2:B:109:LEU:HD22 | 4 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3435) | 1:A:15:ILE:HD11 | 2:B:109:LEU:HD21 | 4 | 1.03 |
| (2,3435) | 1:A:15:ILE:HD13 | 2:B:109:LEU:HD21 | 4 | 1.03 |
| (2,3435) | 1:A:15:ILE:HD11 | 2:B:109:LEU:HD23 | 4 | 1.03 |
| (2,2897) | 2:B:127:LEU:HB3 | 2:B:124:LYS:HD2 | 5 | 1.03 |
| (2,2897) | 2:B:127:LEU:HB2 | 2:B:124:LYS:HD2 | 5 | 1.03 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 1 | 1.02 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 1 | 1.02 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 1 | 1.02 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 2 | 1.01 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 5 | 1.01 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 1 | 1.01 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 8 | 1.01 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 1 | 1.01 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 1 | 1.01 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 1 | 1.01 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 1 | 1.01 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 1 | 1.01 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB2 | 2 | 1.01 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB1 | 2 | 1.01 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB3 | 2 | 1.01 |
| (2,2583) | 1:A:61:CYS:HB3 | 1:A:65:ALA:HB3 | 2 | 1.01 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 7 | 1.01 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 7 | 1.01 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 7 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 1 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 1 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 2 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 2 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 3 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 3 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 4 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 4 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 5 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 5 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 6 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 6 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 7 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 7 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 8 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 8 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 9 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 9 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1714) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HB3 | 10 | 1.01 |
| (2,1714) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HB3 | 10 | 1.01 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 1 | 1.01 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 1 | 1.01 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 5 | 1.0 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 5 | 1.0 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 5 | 1.0 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 5 | 1.0 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 5 | 1.0 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 5 | 1.0 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 7 | 1.0 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 7 | 1.0 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 7 | 1.0 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 7 | 1.0 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 7 | 1.0 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 7 | 1.0 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 10 | 1.0 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 10 | 1.0 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 10 | 1.0 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 10 | 1.0 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 4 | 1.0 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 4 | 1.0 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 4 | 1.0 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 4 | 1.0 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 8 | 0.99 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 8 | 0.99 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 8 | 0.99 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 8 | 0.99 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 8 | 0.99 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 8 | 0.99 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 9 | 0.99 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 10 | 0.99 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 2 | 0.99 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 3 | 0.99 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 2 | 0.99 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 9 | 0.99 |
| (2,2861) | 2:B:124:LYS:HE3 | 2:B:124:LYS:HB2 | 6 | 0.99 |
| (2,2861) | 2:B:124:LYS:HE3 | 2:B:124:LYS:HB3 | 6 | 0.99 |
| (2,951) | 2:B:125:LYS:HD2 | 2:B:129:SER:HB3 | 5 | 0.98 |
| (2,951) | 2:B:125:LYS:HD3 | 2:B:129:SER:HB3 | 5 | 0.98 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 10 | 0.98 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 10 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 10 | 0.98 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 10 | 0.98 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 10 | 0.98 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 10 | 0.98 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 1 | 0.98 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 4 | 0.98 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 5 | 0.98 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 6 | 0.98 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB2 | 5 | 0.98 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB1 | 5 | 0.98 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB3 | 5 | 0.98 |
| (2,2583) | 1:A:61:CYS:HB3 | 1:A:65:ALA:HB3 | 5 | 0.98 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 3 | 0.98 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 3 | 0.98 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB2 | 8 | 0.98 |
| (2,2188) | 1:A:18:ASP:HB2 | 1:A:19:ASP:HB3 | 8 | 0.98 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 8 | 0.98 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 8 | 0.98 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 2 | 0.98 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 2 | 0.98 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.98 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.98 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 4 | 0.97 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 4 | 0.97 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 4 | 0.97 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 4 | 0.97 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 4 | 0.97 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 4 | 0.97 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 1 | 0.97 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 7 | 0.97 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 4 | 0.97 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 5 | 0.97 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 7 | 0.97 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 10 | 0.97 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 10 | 0.97 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 10 | 0.97 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 10 | 0.97 |
| (2,2011) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 0.97 |
| (2,2011) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 0.97 |
| (2,2011) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 0.97 |
| (2,2011) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 0.97 |
| (2,2011) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2011) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 0.97 |
| (2,1936) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 4 | 0.97 |
| (2,1936) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 4 | 0.97 |
| (2,1936) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 4 | 0.97 |
| (2,1642) | 2:B:109:LEU:HA | 2:B:109:LEU:HD12 | 4 | 0.97 |
| (2,1642) | 2:B:109:LEU:HA | 2:B:109:LEU:HD13 | 4 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 4 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 4 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 6 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 6 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 7 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 7 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 8 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 8 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 9 | 0.97 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 9 | 0.97 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 10 | 0.96 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 10 | 0.96 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 10 | 0.96 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 2 | 0.96 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 2 | 0.96 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 2 | 0.96 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 2 | 0.96 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 2 | 0.96 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 2 | 0.96 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 8 | 0.96 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 7 | 0.96 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 10 | 0.96 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 2 | 0.96 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 4 | 0.96 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 4 | 0.96 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 4 | 0.96 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 4 | 0.96 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 4 | 0.96 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 4 | 0.96 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 4 | 0.96 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 4 | 0.96 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 6 | 0.96 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 6 | 0.96 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 6 | 0.96 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 6 | 0.96 |
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD1 | 9 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3023) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HD2 | 9 | 0.96 |
| (2,3023) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HD2 | 9 | 0.96 |
| (2,3023) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HD2 | 9 | 0.96 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 8 | 0.96 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 8 | 0.96 |
| (2,2245) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE3 | 2 | 0.96 |
| (2,2245) | 1:A:24:THR:HG23 | 1:A:27:LYS:HE3 | 2 | 0.96 |
| (2,2245) | 1:A:24:THR:HG21 | 1:A:27:LYS:HE3 | 2 | 0.96 |
| (2,2245) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE2 | 2 | 0.96 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 5 | 0.96 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 5 | 0.96 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 1 | 0.95 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 1 | 0.95 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 1 | 0.95 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 1 | 0.95 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 1 | 0.95 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 1 | 0.95 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 1 | 0.95 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 1 | 0.95 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 1 | 0.95 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 7 | 0.95 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 1 | 0.95 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 1 | 0.95 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 3 | 0.95 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 3 | 0.95 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 3 | 0.95 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 4 | 0.95 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 4 | 0.95 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 3 | 0.95 |
| (2,1208) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 3 | 0.95 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 4 | 0.94 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 3 | 0.94 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 4 | 0.94 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 5 | 0.94 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 6 | 0.94 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 10 | 0.94 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 2 | 0.94 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 3 | 0.94 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 6 | 0.94 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 8 | 0.94 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 7 | 0.94 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 8 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 4 | 0.93 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 6 | 0.93 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 4 | 0.93 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 10 | 0.93 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 10 | 0.93 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 10 | 0.93 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 10 | 0.93 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 1 | 0.93 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 1 | 0.93 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 10 | 0.93 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 10 | 0.93 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 10 | 0.93 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 10 | 0.93 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 8 | 0.92 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 8 | 0.92 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 8 | 0.92 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 6 | 0.92 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 6 | 0.92 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 6 | 0.92 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 9 | 0.92 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 9 | 0.92 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 6 | 0.92 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 6 | 0.92 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 6 | 0.92 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 6 | 0.92 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 6 | 0.92 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 6 | 0.92 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 3 | 0.92 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 3 | 0.92 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 3 | 0.92 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 9 | 0.92 |
| (2,2694) | 2:B:109:LEU:HA | 2:B:109:LEU:HD13 | 4 | 0.92 |
| (2,2694) | 2:B:109:LEU:HA | 2:B:109:LEU:HD12 | 4 | 0.92 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 3 | 0.92 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 3 | 0.92 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 3 | 0.92 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 8 | 0.92 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 8 | 0.92 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 8 | 0.92 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 7 | 0.91 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 8 | 0.91 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 1 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 1 | 0.91 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 1 | 0.91 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 3 | 0.91 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 3 | 0.91 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 10 | 0.91 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 10 | 0.91 |
| (2,1645) | 2:B:109:LEU:HA | 2:B:109:LEU:HD12 | 4 | 0.91 |
| (2,1645) | 2:B:109:LEU:HA | 2:B:109:LEU:HD13 | 4 | 0.91 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 4 | 0.91 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 4 | 0.91 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 3 | 0.9 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 3 | 0.9 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 3 | 0.9 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 3 | 0.9 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 3 | 0.9 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 3 | 0.9 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 3 | 0.9 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 3 | 0.9 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 3 | 0.9 |
| (2,4486) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 2 | 0.9 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 7 | 0.9 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 7 | 0.9 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 7 | 0.9 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 7 | 0.9 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 7 | 0.9 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 1 | 0.9 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 1 | 0.9 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 1 | 0.9 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 1 | 0.9 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 1 | 0.9 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 1 | 0.9 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 2 | 0.9 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 2 | 0.9 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.9 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.9 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 8 | 0.9 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 8 | 0.9 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 8 | 0.9 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 8 | 0.9 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 3 | 0.9 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 3 | 0.9 |
| (2,1746) | 2:B:124:LYS:HE3 | 2:B:124:LYS:HB2 | 6 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1746) | 2:B:124:LYS:HE3 | 2:B:124:LYS:HB3 | 6 | 0.9 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 4 | 0.89 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 4 | 0.89 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD22 | 9 | 0.89 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD21 | 9 | 0.89 |
| (2,770) | 1:A:11:TYR:HD1 | 2:B:112:LEU:HD23 | 9 | 0.89 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD22 | 9 | 0.89 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD21 | 9 | 0.89 |
| (2,770) | 1:A:11:TYR:HD2 | 1:A:14:LEU:HD23 | 9 | 0.89 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 9 | 0.89 |
| (2,4499) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 10 | 0.89 |
| (2,4097) | 2:B:138:ARG:HG3 | 2:B:103:TYR:HE1 | 10 | 0.89 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 0.89 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 10 | 0.89 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 10 | 0.89 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 2 | 0.89 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 2 | 0.89 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 2 | 0.89 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 2 | 0.89 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 2 | 0.89 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 2 | 0.89 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 4 | 0.89 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 4 | 0.89 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 4 | 0.89 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 4 | 0.89 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 4 | 0.89 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 4 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 4 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 4 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 6 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 6 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 7 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 7 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 8 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 8 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 9 | 0.89 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 9 | 0.89 |
| (2,2368) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 3 | 0.89 |
| (2,2368) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 3 | 0.89 |
| (2,2368) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 3 | 0.89 |
| (2,2368) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 3 | 0.89 |
| (2,2368) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 3 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 8 | 0.89 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 8 | 0.89 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 7 | 0.89 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 7 | 0.89 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 1 | 0.89 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 1 | 0.89 |
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 8 | 0.89 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 8 | 0.89 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 8 | 0.89 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 8 | 0.89 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 5 | 0.88 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 5 | 0.88 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 5 | 0.88 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 1 | 0.88 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 1 | 0.88 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 1 | 0.88 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 2 | 0.88 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 2 | 0.88 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 2 | 0.88 |
| (2,752) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 2 | 0.88 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 6 | 0.88 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 6 | 0.88 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 6 | 0.88 |
| (2,752) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 6 | 0.88 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 5 | 0.88 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 6 | 0.88 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 5 | 0.88 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 5 | 0.88 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 5 | 0.88 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 1 | 0.88 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 1 | 0.88 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 1 | 0.88 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 1 | 0.88 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 1 | 0.88 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 1 | 0.88 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 5 | 0.88 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 5 | 0.88 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 1 | 0.88 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 1 | 0.88 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 1 | 0.88 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 7 | 0.88 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 7 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 10 | 0.88 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 10 | 0.88 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 10 | 0.88 |
| (2,1936) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 5 | 0.88 |
| (2,1936) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 5 | 0.88 |
| (2,1936) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 5 | 0.88 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 2 | 0.88 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 2 | 0.88 |
| (2,596) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 3 | 0.87 |
| (2,596) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 3 | 0.87 |
| (2,596) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 3 | 0.87 |
| (2,596) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 3 | 0.87 |
| (2,596) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 3 | 0.87 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 1 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 1 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 2 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 3 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 4 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 5 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 7 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 8 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 9 | 0.87 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 10 | 0.87 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 10 | 0.87 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 2 | 0.87 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 2 | 0.87 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 7 | 0.87 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 8 | 0.87 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 9 | 0.87 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 10 | 0.87 |
| (2,3739) | 1:A:59:LEU:H | 1:A:58:SER:HB3 | 3 | 0.87 |
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 3 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3224) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 3 | 0.87 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 7 | 0.87 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 7 | 0.87 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 7 | 0.87 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 7 | 0.87 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 2 | 0.87 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 2 | 0.87 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 3 | 0.87 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 3 | 0.87 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 3 | 0.87 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 8 | 0.86 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 8 | 0.86 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 6 | 0.86 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 6 | 0.86 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 6 | 0.86 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 3 | 0.86 |
| (2,4372) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 6 | 0.86 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 9 | 0.86 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 3 | 0.86 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 10 | 0.86 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 1 | 0.86 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 1 | 0.86 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 1 | 0.86 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 4 | 0.86 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 4 | 0.86 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 4 | 0.86 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 8 | 0.86 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 8 | 0.86 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 8 | 0.86 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 5 | 0.86 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 5 | 0.86 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 5 | 0.86 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 5 | 0.86 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 5 | 0.86 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 5 | 0.86 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 2 | 0.86 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 2 | 0.86 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 1 | 0.86 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 1 | 0.86 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 1 | 0.86 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 10 | 0.86 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 10 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 10 | 0.86 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 1 | 0.86 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 1 | 0.86 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 7 | 0.86 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 7 | 0.86 |
| (2,1936) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 2 | 0.86 |
| (2,1936) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 2 | 0.86 |
| (2,1936) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 2 | 0.86 |
| (2,1936) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 9 | 0.86 |
| (2,1936) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 9 | 0.86 |
| (2,1936) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 9 | 0.86 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 7 | 0.86 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 7 | 0.86 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 2 | 0.86 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 2 | 0.86 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.86 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.86 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 4 | 0.85 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 4 | 0.85 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 7 | 0.85 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 7 | 0.85 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 2 | 0.85 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 2 | 0.85 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 2 | 0.85 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 7 | 0.85 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 7 | 0.85 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 7 | 0.85 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 3 | 0.85 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 3 | 0.85 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 3 | 0.85 |
| (2,752) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 3 | 0.85 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 2 | 0.85 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 2 | 0.85 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 2 | 0.85 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 2 | 0.85 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 6 | 0.85 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 6 | 0.85 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 3 | 0.85 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 4 | 0.85 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 5 | 0.85 |
| (2,3786) | 2:B:109:LEU:H | 1:A:11:TYR:HD1 | 4 | 0.85 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 2 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 2 | 0.85 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 2 | 0.85 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 7 | 0.85 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 7 | 0.85 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 7 | 0.85 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 7 | 0.85 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 7 | 0.85 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 7 | 0.85 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 7 | 0.85 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 9 | 0.85 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 9 | 0.85 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 9 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 4 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 4 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 6 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 6 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 7 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 7 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 8 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 8 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 9 | 0.85 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 9 | 0.85 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 7 | 0.84 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 7 | 0.84 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 7 | 0.84 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 4 | 0.84 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 4 | 0.84 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 4 | 0.84 |
| (2,752) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 4 | 0.84 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 3 | 0.84 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 3 | 0.84 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 3 | 0.84 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 3 | 0.84 |
| (2,4521) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 8 | 0.84 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 2 | 0.84 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 1 | 0.84 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 2 | 0.84 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 1 | 0.84 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 1 | 0.84 |
| (2,3834) | 2:B:121:LYS:H | 2:B:121:LYS:HB3 | 6 | 0.84 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 9 | 0.84 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 9 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 9 | 0.84 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 9 | 0.84 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 9 | 0.84 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 9 | 0.84 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 8 | 0.84 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 8 | 0.84 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 5 | 0.84 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 5 | 0.84 |
| (2,841) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 9 | 0.83 |
| (2,841) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 9 | 0.83 |
| (2,841) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 9 | 0.83 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 5 | 0.83 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 5 | 0.83 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 7 | 0.83 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 5 | 0.83 |
| (2,3962) | 2:B:144:SER:H | 2:B:143:ILE:HG12 | 3 | 0.83 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 8 | 0.83 |
| (2,3739) | 1:A:59:LEU:H | 1:A:58:SER:HB3 | 5 | 0.83 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 3 | 0.83 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 3 | 0.83 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 3 | 0.83 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 6 | 0.83 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 6 | 0.83 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 6 | 0.83 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 3 | 0.83 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 3 | 0.83 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 3 | 0.83 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 3 | 0.83 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 3 | 0.83 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 3 | 0.83 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 8 | 0.83 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 8 | 0.83 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 8 | 0.83 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 8 | 0.83 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 9 | 0.83 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 9 | 0.83 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 4 | 0.83 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 4 | 0.83 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 3 | 0.83 |
| (2,1200) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 3 | 0.83 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 1 | 0.82 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 1 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 1 | 0.82 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 1 | 0.82 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 2 | 0.82 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 3 | 0.82 |
| (2,4414) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 8 | 0.82 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 4 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 1 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 2 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 3 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 4 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 5 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 7 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 8 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 9 | 0.82 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 10 | 0.82 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 7 | 0.82 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 5 | 0.82 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 5 | 0.82 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 5 | 0.82 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 4 | 0.82 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 4 | 0.82 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 4 | 0.82 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 4 | 0.82 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 10 | 0.82 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 10 | 0.82 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 10 | 0.82 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 3 | 0.82 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 3 | 0.82 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 3 | 0.82 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 3 | 0.82 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 3 | 0.82 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 3 | 0.82 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 1 | 0.82 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 1 | 0.82 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 3 | 0.82 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 3 | 0.82 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 6 | 0.82 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 6 | 0.82 |
| (2,2022) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 0.82 |
| (2,2022) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 0.82 |
| (2,2022) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 0.82 |
| (2,2022) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2022) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 0.82 |
| (2,2022) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 0.82 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 10 | 0.82 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 10 | 0.82 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 10 | 0.82 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 10 | 0.82 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 10 | 0.82 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 10 | 0.82 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 10 | 0.82 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 10 | 0.82 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 10 | 0.82 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 3 | 0.82 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 3 | 0.82 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 3 | 0.82 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 3 | 0.82 |
| (2,1063) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 3 | 0.82 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 5 | 0.81 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 10 | 0.81 |
| (2,4222) | 1:A:4:VAL:HB | 1:A:3:SER:HB3 | 5 | 0.81 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 2 | 0.81 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 9 | 0.81 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 10 | 0.81 |
| (2,4048) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 6 | 0.81 |
| (2,4008) | 1:A:4:VAL:HB | 1:A:3:SER:HB3 | 5 | 0.81 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 3 | 0.81 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 4 | 0.81 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 5 | 0.81 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 6 | 0.81 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 10 | 0.81 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 9 | 0.81 |
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 9 | 0.81 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 9 | 0.81 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG12 | 4 | 0.81 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG13 | 4 | 0.81 |
| (2,3509) | 2:B:159:ILE:HG23 | 1:A:10:ILE:HG13 | 4 | 0.81 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG12 | 4 | 0.81 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG13 | 4 | 0.81 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 1 | 0.81 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 1 | 0.81 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 1 | 0.81 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 6 | 0.81 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 6 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 6 | 0.81 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 5 | 0.81 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 5 | 0.81 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 4 | 0.81 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 4 | 0.81 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 5 | 0.81 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 5 | 0.81 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 10 | 0.81 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 10 | 0.81 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 3 | 0.81 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 3 | 0.81 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 9 | 0.81 |
| (2,1929) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 9 | 0.81 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 5 | 0.81 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 5 | 0.81 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 7 | 0.81 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 7 | 0.81 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 6 | 0.81 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 6 | 0.81 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 6 | 0.81 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 6 | 0.81 |
| (2,1063) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 6 | 0.81 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 2 | 0.8 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 2 | 0.8 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 5 | 0.8 |
| (2,4084) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 5 | 0.8 |
| (2,3962) | 2:B:144:SER:H | 2:B:143:ILE:HG12 | 4 | 0.8 |
| (2,3739) | 1:A:59:LEU:H | 1:A:58:SER:HB3 | 8 | 0.8 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 3 | 0.8 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 3 | 0.8 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 3 | 0.8 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 2 | 0.8 |
| (2,2569) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 2 | 0.8 |
| (2,2318) | 1:A:32:ILE:HD12 | 1:A:9:CYS:H | 3 | 0.8 |
| (2,2318) | 1:A:32:ILE:HD13 | 1:A:9:CYS:H | 3 | 0.8 |
| (2,1824) | 2:B:134:ALA:HB2 | 2:B:124:LYS:HE2 | 6 | 0.8 |
| (2,1824) | 2:B:134:ALA:HB1 | 2:B:124:LYS:HE2 | 6 | 0.8 |
| (2,1824) | 2:B:134:ALA:HB3 | 2:B:124:LYS:HE2 | 6 | 0.8 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 2 | 0.8 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 2 | 0.8 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 2 | 0.8 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 2 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1063) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 2 | 0.8 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 9 | 0.79 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 9 | 0.79 |
| (2,4222) | 1:A:4:VAL:HB | 1:A:3:SER:HB3 | 10 | 0.79 |
| (2,4008) | 1:A:4:VAL:HB | 1:A:3:SER:HB3 | 10 | 0.79 |
| (2,3962) | 2:B:144:SER:H | 2:B:143:ILE:HG12 | 1 | 0.79 |
| (2,3962) | 2:B:144:SER:H | 2:B:143:ILE:HG12 | 10 | 0.79 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 6 | 0.79 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 6 | 0.79 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 6 | 0.79 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 6 | 0.79 |
| (2,3315) | 1:A:8:ALA:HB2 | 2:B:109:LEU:HD12 | 4 | 0.79 |
| (2,3315) | 1:A:8:ALA:HB2 | 2:B:109:LEU:HD11 | 4 | 0.79 |
| (2,3315) | 1:A:8:ALA:HB2 | 2:B:109:LEU:HD13 | 4 | 0.79 |
| (2,3315) | 1:A:8:ALA:HB1 | 2:B:109:LEU:HD12 | 4 | 0.79 |
| (2,3315) | 1:A:8:ALA:HB1 | 2:B:109:LEU:HD11 | 4 | 0.79 |
| (2,3315) | 1:A:8:ALA:HB1 | 2:B:109:LEU:HD13 | 4 | 0.79 |
| (2,3273) | 2:B:165:VAL:HA | 2:B:165:VAL:HG12 | 7 | 0.79 |
| (2,3273) | 2:B:165:VAL:HA | 2:B:165:VAL:HG11 | 7 | 0.79 |
| (2,3273) | 2:B:165:VAL:HA | 2:B:165:VAL:HG13 | 7 | 0.79 |
| (2,3273) | 2:B:165:VAL:HA | 2:B:165:VAL:HG22 | 7 | 0.79 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 4 | 0.79 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 4 | 0.79 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 4 | 0.79 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 4 | 0.79 |
| (2,3072) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 3 | 0.79 |
| (2,3072) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 3 | 0.79 |
| (2,3072) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 3 | 0.79 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 5 | 0.79 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 5 | 0.79 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 5 | 0.79 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 5 | 0.79 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 5 | 0.79 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 10 | 0.79 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 10 | 0.79 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 10 | 0.79 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 6 | 0.79 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 6 | 0.79 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 1 | 0.79 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 1 | 0.79 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 1 | 0.79 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 5 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 5 | 0.78 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 5 | 0.78 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 6 | 0.78 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 6 | 0.78 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 6 | 0.78 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 3 | 0.78 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 7 | 0.78 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 3 | 0.78 |
| (2,3857) | 2:B:125:LYS:H | 2:B:125:LYS:HE3 | 4 | 0.78 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 8 | 0.78 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 8 | 0.78 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 8 | 0.78 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 8 | 0.78 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 8 | 0.78 |
| (2,3387) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 3 | 0.78 |
| (2,3387) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 3 | 0.78 |
| (2,3387) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 3 | 0.78 |
| (2,3387) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 3 | 0.78 |
| (2,3387) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 3 | 0.78 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 7 | 0.78 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 7 | 0.78 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 7 | 0.78 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 7 | 0.78 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 10 | 0.78 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 10 | 0.78 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 7 | 0.78 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 7 | 0.78 |
| (2,2626) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 7 | 0.78 |
| (2,2626) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 7 | 0.78 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 6 | 0.78 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 6 | 0.78 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 6 | 0.78 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 5 | 0.78 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 5 | 0.78 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 5 | 0.78 |
| (2,2368) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 1 | 0.78 |
| (2,2368) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 1 | 0.78 |
| (2,2368) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 1 | 0.78 |
| (2,2368) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 1 | 0.78 |
| (2,2368) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 1 | 0.78 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG22 | 8 | 0.78 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG21 | 8 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG23 | 8 | 0.78 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG12 | 8 | 0.78 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG11 | 8 | 0.78 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG22 | 8 | 0.78 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG21 | 8 | 0.78 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG23 | 8 | 0.78 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 7 | 0.78 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 7 | 0.78 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 7 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 2 | 0.78 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 2 | 0.78 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 2 | 0.78 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 2 | 0.78 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 2 | 0.78 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 2 | 0.78 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 2 | 0.78 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 2 | 0.78 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 2 | 0.78 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 2 | 0.78 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 2 | 0.78 |
| (2,1245) | 2:B:165:VAL:HA | 2:B:165:VAL:HG12 | 7 | 0.78 |
| (2,1245) | 2:B:165:VAL:HA | 2:B:165:VAL:HG11 | 7 | 0.78 |
| (2,1245) | 2:B:165:VAL:HA | 2:B:165:VAL:HG13 | 7 | 0.78 |
| (2,1245) | 2:B:165:VAL:HA | 2:B:165:VAL:HG22 | 7 | 0.78 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 3 | 0.77 |
| (2,4140) | 1:A:27:LYS:HA | 1:A:27:LYS:HE2 | 2 | 0.77 |
| (2,3911) | 2:B:133:GLU:H | 2:B:133:GLU:HB3 | 2 | 0.77 |
| (2,3281) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 0.77 |
| (2,3281) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 0.77 |
| (2,3281) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 0.77 |
| (2,3281) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 0.77 |
| (2,3281) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 0.77 |
| (2,3281) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3074) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD13 | 4 | 0.77 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD12 | 4 | 0.77 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD11 | 4 | 0.77 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD13 | 4 | 0.77 |
| (2,3074) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD12 | 4 | 0.77 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 4 | 0.77 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 4 | 0.77 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 8 | 0.77 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 8 | 0.77 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 3 | 0.77 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 3 | 0.77 |
| (2,1105) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD12 | 4 | 0.77 |
| (2,1105) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD13 | 4 | 0.77 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD12 | 4 | 0.77 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD11 | 4 | 0.77 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD13 | 4 | 0.77 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 1 | 0.76 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 1 | 0.76 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 6 | 0.76 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 6 | 0.76 |
| (2,596) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 1 | 0.76 |
| (2,596) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 1 | 0.76 |
| (2,596) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 1 | 0.76 |
| (2,596) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 1 | 0.76 |
| (2,596) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 1 | 0.76 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 1 | 0.76 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 1 | 0.76 |
| (2,3857) | 2:B:125:LYS:H | 2:B:125:LYS:HE3 | 8 | 0.76 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 1 | 0.76 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 1 | 0.76 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 8 | 0.76 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 7 | 0.76 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 7 | 0.76 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 7 | 0.76 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 1 | 0.76 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 1 | 0.76 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 1 | 0.76 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 1 | 0.76 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 3 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 3 | 0.76 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 3 | 0.76 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 1 | 0.76 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 1 | 0.76 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 1 | 0.76 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 9 | 0.76 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 9 | 0.76 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 4 | 0.76 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 4 | 0.76 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 4 | 0.76 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 4 | 0.76 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 4 | 0.76 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 4 | 0.76 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 4 | 0.76 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 4 | 0.76 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 4 | 0.76 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 9 | 0.76 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 9 | 0.76 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 8 | 0.76 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 8 | 0.76 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 8 | 0.76 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 8 | 0.76 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 8 | 0.76 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 7 | 0.76 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 7 | 0.76 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,1063) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 7 | 0.76 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 1 | 0.75 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 1 | 0.75 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 8 | 0.75 |
| (2,4170) | 1:A:43:TRP:HA | 1:A:46:LEU:HB2 | 3 | 0.75 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 3 | 0.75 |
| (2,3857) | 2:B:125:LYS:H | 2:B:125:LYS:HE3 | 9 | 0.75 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 3 | 0.75 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 3 | 0.75 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 8 | 0.75 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 8 | 0.75 |
| (2,369) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 6 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,369) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 6 | 0.75 |
| (2,369) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 6 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 2 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 2 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 2 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 3 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 3 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 3 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 8 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 8 | 0.75 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 8 | 0.75 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 6 | 0.75 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 6 | 0.75 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 6 | 0.75 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 6 | 0.75 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 4 | 0.75 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 4 | 0.75 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 4 | 0.75 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 4 | 0.75 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB2 | 7 | 0.75 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB1 | 7 | 0.75 |
| (2,2583) | 1:A:61:CYS:HB2 | 1:A:65:ALA:HB3 | 7 | 0.75 |
| (2,2583) | 1:A:61:CYS:HB3 | 1:A:65:ALA:HB3 | 7 | 0.75 |
| (2,1643) | 2:B:109:LEU:HA | 2:B:109:LEU:HD12 | 4 | 0.75 |
| (2,1643) | 2:B:109:LEU:HA | 2:B:109:LEU:HD13 | 4 | 0.75 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 1 | 0.75 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 1 | 0.75 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 3 | 0.75 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 3 | 0.75 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 6 | 0.75 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 6 | 0.75 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 10 | 0.75 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 10 | 0.75 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 3 | 0.74 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 3 | 0.74 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 3 | 0.74 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 5 | 0.74 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 5 | 0.74 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 5 | 0.74 |
| (2,752) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 5 | 0.74 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 7 | 0.74 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 9 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 9 | 0.74 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 6 | 0.74 |
| (2,385) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 6 | 0.74 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 4 | 0.74 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 4 | 0.74 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 4 | 0.74 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 9 | 0.74 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 9 | 0.74 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 9 | 0.74 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 9 | 0.74 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 5 | 0.74 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 5 | 0.74 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 5 | 0.74 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 7 | 0.74 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 7 | 0.74 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 7 | 0.74 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 1 | 0.74 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 1 | 0.74 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 3 | 0.74 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 3 | 0.74 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 3 | 0.74 |
| (2,2580) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 2 | 0.74 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 2 | 0.74 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 2 | 0.74 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 2 | 0.74 |
| (2,2580) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 6 | 0.74 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 6 | 0.74 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 6 | 0.74 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 6 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 4 | 0.74 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 4 | 0.74 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 4 | 0.74 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 4 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 5 | 0.74 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 5 | 0.74 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 10 | 0.74 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 10 | 0.74 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 2 | 0.74 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 2 | 0.74 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 1 | 0.73 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 1 | 0.73 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 1 | 0.73 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 5 | 0.73 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 5 | 0.73 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 5 | 0.73 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 3 | 0.73 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 1 | 0.73 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 2 | 0.73 |
| (2,3857) | 2:B:125:LYS:H | 2:B:125:LYS:HE3 | 6 | 0.73 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 5 | 0.73 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 5 | 0.73 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 5 | 0.73 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 5 | 0.73 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 8 | 0.73 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 8 | 0.73 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 9 | 0.73 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 9 | 0.73 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 9 | 0.73 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 9 | 0.73 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 9 | 0.73 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 6 | 0.73 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 6 | 0.73 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 3 | 0.73 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 3 | 0.73 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 3 | 0.73 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 3 | 0.73 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 3 | 0.73 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 3 | 0.73 |
| (2,2318) | 1:A:32:ILE:HD12 | 1:A:9:CYS:H | 5 | 0.73 |
| (2,2318) | 1:A:32:ILE:HD13 | 1:A:9:CYS:H | 5 | 0.73 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 2 | 0.73 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 2 | 0.73 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB3 | 3 | 0.73 |
| (2,1994) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HB3 | 3 | 0.73 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB2 | 3 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 4 | 0.73 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 4 | 0.73 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 4 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 1 | 0.73 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 1 | 0.73 |
| (2,1594) | 1:A:60:ILE:HD12 | 1:A:60:ILE:HG22 | 6 | 0.73 |
| (2,1594) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HG22 | 6 | 0.73 |
| (2,1594) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HG21 | 6 | 0.73 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG22 | 6 | 0.73 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG21 | 6 | 0.73 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG23 | 6 | 0.73 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD11 | 2 | 0.73 |
| (2,152) | 1:A:60:ILE:H | 1:A:60:ILE:HD13 | 2 | 0.73 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 1 | 0.73 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 1 | 0.73 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 7 | 0.73 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 7 | 0.73 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 4 | 0.72 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 4 | 0.72 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 4 | 0.72 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 2 | 0.72 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 2 | 0.72 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 2 | 0.72 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 7 | 0.72 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 7 | 0.72 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 7 | 0.72 |
| (2,4451) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 8 | 0.72 |
| (2,4082) | 2:B:123:ILE:HD12 | 2:B:107:TYR:HD2 | 8 | 0.72 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 6 | 0.72 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 6 | 0.72 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 6 | 0.72 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 10 | 0.72 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 10 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 10 | 0.72 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 10 | 0.72 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 1 | 0.72 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 1 | 0.72 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 1 | 0.72 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 1 | 0.72 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 1 | 0.72 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 1 | 0.72 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 1 | 0.72 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 1 | 0.72 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 4 | 0.72 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 4 | 0.72 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 4 | 0.72 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 4 | 0.72 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 4 | 0.72 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 7 | 0.72 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 7 | 0.72 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 3 | 0.72 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 3 | 0.72 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 3 | 0.72 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 3 | 0.72 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 8 | 0.72 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 8 | 0.72 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 8 | 0.72 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 3 | 0.72 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 3 | 0.72 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 3 | 0.72 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 3 | 0.72 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 3 | 0.72 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 3 | 0.72 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 3 | 0.72 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 3 | 0.72 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 3 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD12 | 1:A:60:ILE:HG22 | 1 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HG22 | 1 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HG21 | 1 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG22 | 1 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG21 | 1 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG23 | 1 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD12 | 1:A:60:ILE:HG22 | 7 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HG22 | 7 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HG21 | 7 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG22 | 7 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG21 | 7 | 0.72 |
| (2,1594) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HG23 | 7 | 0.72 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 5 | 0.71 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 5 | 0.71 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 10 | 0.71 |
| (2,880) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 10 | 0.71 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 4 | 0.71 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 4 | 0.71 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 4 | 0.71 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 7 | 0.71 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 7 | 0.71 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 7 | 0.71 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 3 | 0.71 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 3 | 0.71 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 3 | 0.71 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 9 | 0.71 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 9 | 0.71 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 9 | 0.71 |
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 6 | 0.71 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 6 | 0.71 |
| (2,4195) | 2:B:149:LYS:HA | 2:B:149:LYS:HD2 | 8 | 0.71 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 9 | 0.71 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 9 | 0.71 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 9 | 0.71 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 10 | 0.71 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 10 | 0.71 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 10 | 0.71 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 2 | 0.71 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 2 | 0.71 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 2 | 0.71 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 2 | 0.71 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 2 | 0.71 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.71 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.71 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 10 | 0.71 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 10 | 0.71 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 10 | 0.71 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 10 | 0.71 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 7 | 0.71 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 7 | 0.71 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 7 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2580) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 3 | 0.71 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 3 | 0.71 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 3 | 0.71 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 3 | 0.71 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD2 | 4 | 0.71 |
| (2,2488) | 1:A:51:LEU:HB2 | 1:A:47:PHE:HD1 | 4 | 0.71 |
| (2,2488) | 1:A:51:LEU:HB3 | 1:A:47:PHE:HD1 | 4 | 0.71 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 10 | 0.71 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 10 | 0.71 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG22 | 4 | 0.71 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG21 | 4 | 0.71 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG23 | 4 | 0.71 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG12 | 4 | 0.71 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG11 | 4 | 0.71 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG22 | 4 | 0.71 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG21 | 4 | 0.71 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG23 | 4 | 0.71 |
| (2,951) | 2:B:125:LYS:HD2 | 2:B:129:SER:HB3 | 10 | 0.7 |
| (2,951) | 2:B:125:LYS:HD3 | 2:B:129:SER:HB3 | 10 | 0.7 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 10 | 0.7 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 10 | 0.7 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 10 | 0.7 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.7 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.7 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.7 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 7 | 0.7 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 7 | 0.7 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 7 | 0.7 |
| (2,752) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 7 | 0.7 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 7 | 0.7 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 7 | 0.7 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 7 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 4 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 4 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 6 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 6 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 7 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 7 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 8 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 8 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 9 | 0.7 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 9 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 10 | 0.7 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 10 | 0.7 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 9 | 0.7 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 9 | 0.7 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 10 | 0.7 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 10 | 0.7 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 10 | 0.7 |
| (2,2580) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 4 | 0.7 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 4 | 0.7 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 4 | 0.7 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 4 | 0.7 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 5 | 0.7 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 5 | 0.7 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 5 | 0.7 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 5 | 0.7 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 4 | 0.7 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 4 | 0.7 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 4 | 0.7 |
| (2,2318) | 1:A:32:ILE:HD12 | 1:A:9:CYS:H | 9 | 0.7 |
| (2,2318) | 1:A:32:ILE:HD13 | 1:A:9:CYS:H | 9 | 0.7 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 8 | 0.7 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 8 | 0.7 |
| (2,2008) | 2:B:165:VAL:HA | 2:B:165:VAL:HG12 | 7 | 0.7 |
| (2,2008) | 2:B:165:VAL:HA | 2:B:165:VAL:HG11 | 7 | 0.7 |
| (2,2008) | 2:B:165:VAL:HA | 2:B:165:VAL:HG13 | 7 | 0.7 |
| (2,2008) | 2:B:165:VAL:HA | 2:B:165:VAL:HG22 | 7 | 0.7 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 9 | 0.7 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 9 | 0.7 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 3 | 0.7 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 3 | 0.7 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 4 | 0.7 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 4 | 0.7 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 8 | 0.7 |
| (2,1063) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 8 | 0.7 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 8 | 0.7 |
| (2,1063) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 8 | 0.7 |
| (2,1063) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 8 | 0.7 |
| (2,792) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 10 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 10 | 0.69 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 10 | 0.69 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 1 | 0.69 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 1 | 0.69 |
| (2,3437) | 2:B:109:LEU:HD12 | 1:A:11:TYR:HD1 | 9 | 0.69 |
| (2,3437) | 2:B:109:LEU:HD11 | 1:A:11:TYR:HD1 | 9 | 0.69 |
| (2,3437) | 2:B:109:LEU:HD13 | 1:A:11:TYR:HD1 | 9 | 0.69 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 5 | 0.69 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 5 | 0.69 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 4 | 0.69 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 4 | 0.69 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 8 | 0.69 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 8 | 0.69 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 8 | 0.69 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 9 | 0.69 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 9 | 0.69 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 9 | 0.69 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 9 | 0.69 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 4 | 0.69 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 4 | 0.69 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 4 | 0.69 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 4 | 0.69 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 4 | 0.69 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 1 | 0.69 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 1 | 0.69 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 1 | 0.69 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 1 | 0.69 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 1 | 0.69 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 1 | 0.69 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 1 | 0.69 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 10 | 0.69 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 10 | 0.69 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 10 | 0.69 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 5 | 0.69 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 5 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 5 | 0.69 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 5 | 0.69 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 5 | 0.69 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 5 | 0.69 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 5 | 0.69 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 5 | 0.69 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 5 | 0.69 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 8 | 0.69 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 8 | 0.69 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 1 | 0.69 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 1 | 0.69 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 2 | 0.68 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 2 | 0.68 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 2 | 0.68 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 10 | 0.68 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 10 | 0.68 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 10 | 0.68 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 10 | 0.68 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 3 | 0.68 |
| (2,3213) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 3 | 0.68 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 8 | 0.68 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 8 | 0.68 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 8 | 0.68 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 8 | 0.68 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 8 | 0.68 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 8 | 0.68 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 8 | 0.68 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 9 | 0.68 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 9 | 0.68 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 3 | 0.68 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 3 | 0.68 |
| (2,2626) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 3 | 0.68 |
| (2,2626) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 3 | 0.68 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 7 | 0.68 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 7 | 0.68 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 3 | 0.68 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 3 | 0.68 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 8 | 0.68 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 8 | 0.68 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 6 | 0.68 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 6 | 0.68 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 6 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 6 | 0.68 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 6 | 0.68 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 6 | 0.68 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 6 | 0.68 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 6 | 0.68 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 6 | 0.68 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 10 | 0.68 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 10 | 0.68 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 9 | 0.67 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 9 | 0.67 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 9 | 0.67 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 9 | 0.67 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 9 | 0.67 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 6 | 0.67 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 6 | 0.67 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 4 | 0.67 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 5 | 0.67 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 5 | 0.67 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 5 | 0.67 |
| (2,3387) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 1 | 0.67 |
| (2,3387) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 1 | 0.67 |
| (2,3387) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 1 | 0.67 |
| (2,3387) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 1 | 0.67 |
| (2,3387) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 1 | 0.67 |
| (2,2974) | 2:B:134:ALA:HB2 | 2:B:124:LYS:HE2 | 6 | 0.67 |
| (2,2974) | 2:B:134:ALA:HB1 | 2:B:124:LYS:HE2 | 6 | 0.67 |
| (2,2974) | 2:B:134:ALA:HB3 | 2:B:124:LYS:HE2 | 6 | 0.67 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 2 | 0.67 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 2 | 0.67 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 2 | 0.67 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 2 | 0.67 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 2 | 0.67 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 2 | 0.67 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 2 | 0.67 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 6 | 0.67 |
| (2,2096) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 6 | 0.67 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB3 | 8 | 0.67 |
| (2,1994) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HB3 | 8 | 0.67 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB2 | 8 | 0.67 |
| (2,1874) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD12 | 4 | 0.67 |
| (2,1874) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD12 | 4 | 0.67 |
| (2,1874) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD11 | 4 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1874) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD13 | 4 | 0.67 |
| (2,1874) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD13 | 4 | 0.67 |
| (2,1745) | 2:B:134:ALA:HB2 | 2:B:124:LYS:HE2 | 6 | 0.67 |
| (2,1745) | 2:B:134:ALA:HB1 | 2:B:124:LYS:HE2 | 6 | 0.67 |
| (2,1745) | 2:B:134:ALA:HB3 | 2:B:124:LYS:HE2 | 6 | 0.67 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 4 | 0.67 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 4 | 0.67 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 2 | 0.67 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 2 | 0.67 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 4 | 0.66 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 4 | 0.66 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 4 | 0.66 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 4 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 1 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 2 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 3 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 4 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 5 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 7 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 8 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 9 | 0.66 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 10 | 0.66 |
| (2,3857) | 2:B:125:LYS:H | 2:B:125:LYS:HE3 | 2 | 0.66 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 3 | 0.66 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 3 | 0.66 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 3 | 0.66 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 3 | 0.66 |
| (2,3221) | 2:B:159:ILE:HD12 | 2:B:158:GLY:H | 8 | 0.66 |
| (2,3221) | 2:B:159:ILE:HD13 | 2:B:158:GLY:H | 8 | 0.66 |
| (2,3221) | 2:B:159:ILE:HD12 | 1:A:61:CYS:H | 8 | 0.66 |
| (2,3221) | 2:B:159:ILE:HD13 | 1:A:61:CYS:H | 8 | 0.66 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 2 | 0.66 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 2 | 0.66 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 3 | 0.66 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 3 | 0.66 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 4 | 0.66 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 4 | 0.66 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 9 | 0.66 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 9 | 0.66 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 6 | 0.66 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 6 | 0.66 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 6 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 1 | 0.66 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 1 | 0.66 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 1 | 0.66 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 5 | 0.66 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 5 | 0.66 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 5 | 0.66 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 5 | 0.66 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 5 | 0.66 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD12 | 6 | 0.66 |
| (2,219) | 2:B:117:SER:H | 2:B:151:ILE:HD11 | 6 | 0.66 |
| (2,2076) | 1:A:8:ALA:HA | 2:B:109:LEU:HD12 | 4 | 0.66 |
| (2,2076) | 1:A:8:ALA:HA | 2:B:109:LEU:HD11 | 4 | 0.66 |
| (2,2076) | 1:A:8:ALA:HA | 2:B:109:LEU:HD13 | 4 | 0.66 |
| (2,1849) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HD2 | 5 | 0.66 |
| (2,1849) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HD2 | 5 | 0.66 |
| (2,1849) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HD2 | 5 | 0.66 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 1 | 0.66 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 1 | 0.66 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 7 | 0.66 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 7 | 0.66 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 6 | 0.66 |
| (2,1371) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 6 | 0.66 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 3 | 0.66 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 3 | 0.66 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 3 | 0.66 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 2 | 0.65 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 2 | 0.65 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 2 | 0.65 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 3 | 0.65 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 3 | 0.65 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 3 | 0.65 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 8 | 0.65 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 8 | 0.65 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 8 | 0.65 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 8 | 0.65 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 8 | 0.65 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 8 | 0.65 |
| (2,4374) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 6 | 0.65 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 5 | 0.65 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 4 | 0.65 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 4 | 0.65 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 4 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 4 | 0.65 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 2 | 0.65 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 2 | 0.65 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 2 | 0.65 |
| (2,3101) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 2 | 0.65 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 8 | 0.65 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 8 | 0.65 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 8 | 0.65 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 8 | 0.65 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 2 | 0.65 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 2 | 0.65 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 2 | 0.65 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 4 | 0.65 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 4 | 0.65 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 1 | 0.65 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 1 | 0.65 |
| (2,2626) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 1 | 0.65 |
| (2,2626) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 1 | 0.65 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 2 | 0.65 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 2 | 0.65 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 2 | 0.65 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 7 | 0.65 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 7 | 0.65 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 7 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 9 | 0.65 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 9 | 0.65 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 8 | 0.65 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 8 | 0.65 |
| (2,1060) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HD2 | 8 | 0.65 |
| (2,1060) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HD2 | 8 | 0.65 |
| (2,1060) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HD2 | 8 | 0.65 |
| (2,824) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 9 | 0.64 |
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 9 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,824) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 9 | 0.64 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 5 | 0.64 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 5 | 0.64 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 5 | 0.64 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 8 | 0.64 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 8 | 0.64 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 8 | 0.64 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 8 | 0.64 |
| (2,4456) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 5 | 0.64 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 4 | 0.64 |
| (2,4080) | 2:B:122:ASP:HA | 2:B:125:LYS:HB2 | 5 | 0.64 |
| (2,3267) | 2:B:165:VAL:HA | 2:B:165:VAL:HG12 | 7 | 0.64 |
| (2,3267) | 2:B:165:VAL:HA | 2:B:165:VAL:HG11 | 7 | 0.64 |
| (2,3267) | 2:B:165:VAL:HA | 2:B:165:VAL:HG13 | 7 | 0.64 |
| (2,3267) | 2:B:165:VAL:HA | 2:B:165:VAL:HG22 | 7 | 0.64 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 9 | 0.64 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 9 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 5 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 5 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 5 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 5 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 5 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 8 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 8 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 8 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 8 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 8 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 10 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 10 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 10 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 10 | 0.64 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 10 | 0.64 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 8 | 0.64 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 8 | 0.64 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 5 | 0.64 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 5 | 0.64 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 5 | 0.64 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 3 | 0.64 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 3 | 0.64 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 3 | 0.64 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 9 | 0.64 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 9 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 9 | 0.64 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB3 | 2 | 0.64 |
| (2,1994) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HB3 | 2 | 0.64 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB2 | 2 | 0.64 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD12 | 6 | 0.64 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD11 | 6 | 0.64 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD13 | 6 | 0.64 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD12 | 6 | 0.64 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD11 | 6 | 0.64 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD13 | 6 | 0.64 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD21 | 6 | 0.64 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD23 | 6 | 0.64 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 9 | 0.64 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 9 | 0.64 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 9 | 0.64 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 9 | 0.64 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 8 | 0.64 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 8 | 0.64 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 8 | 0.64 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 8 | 0.64 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 8 | 0.64 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 8 | 0.64 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 8 | 0.64 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 8 | 0.64 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 4 | 0.63 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 4 | 0.63 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 4 | 0.63 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 4 | 0.63 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 4 | 0.63 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 5 | 0.63 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 6 | 0.63 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 8 | 0.63 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 10 | 0.63 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 1 | 0.63 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 1 | 0.63 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 6 | 0.63 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 6 | 0.63 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 9 | 0.63 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 9 | 0.63 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 9 | 0.63 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 4 | 0.63 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 4 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,950) | 2:B:125:LYS:HB2 | 2:B:122:ASP:HB2 | 5 | 0.62 |
| (2,950) | 2:B:125:LYS:HB2 | 2:B:122:ASP:HB3 | 5 | 0.62 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 7 | 0.62 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 7 | 0.62 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 7 | 0.62 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 7 | 0.62 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 3 | 0.62 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 3 | 0.62 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 3 | 0.62 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 6 | 0.62 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 6 | 0.62 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 6 | 0.62 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 6 | 0.62 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 6 | 0.62 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 8 | 0.62 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 8 | 0.62 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 8 | 0.62 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 8 | 0.62 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 1 | 0.62 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 1 | 0.62 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 1 | 0.62 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 1 | 0.62 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 8 | 0.62 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 8 | 0.62 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 8 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 1 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 1 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 1 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 1 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 8 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 8 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 8 | 0.62 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 8 | 0.62 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 2 | 0.62 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 2 | 0.62 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 4 | 0.62 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 4 | 0.62 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 2 | 0.61 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 2 | 0.61 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 2 | 0.61 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 2 | 0.61 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 2 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4533) | 2:B:151:ILE:HD13 | 2:B:150:ASN:H | 8 | 0.61 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 4 | 0.61 |
| (2,3855) | 2:B:124:LYS:H | 2:B:124:LYS:HD2 | 5 | 0.61 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 5 | 0.61 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 5 | 0.61 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 10 | 0.61 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 10 | 0.61 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 10 | 0.61 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 10 | 0.61 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 10 | 0.61 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 10 | 0.61 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 10 | 0.61 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 10 | 0.61 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 0.61 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 10 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 3 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 3 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 3 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 3 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 4 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 4 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 4 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 4 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 5 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 5 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 5 | 0.61 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 5 | 0.61 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 3 | 0.61 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 3 | 0.61 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 10 | 0.6 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 10 | 0.6 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 10 | 0.6 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 10 | 0.6 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 2 | 0.6 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 7 | 0.6 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 6 | 0.6 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 9 | 0.6 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 9 | 0.6 |
| (2,3454) | 1:A:35:ALA:HB2 | 2:B:126:ILE:HD12 | 2 | 0.6 |
| (2,3454) | 1:A:35:ALA:HB1 | 2:B:126:ILE:HD12 | 2 | 0.6 |
| (2,3454) | 1:A:35:ALA:HB1 | 2:B:126:ILE:HD11 | 2 | 0.6 |
| (2,3454) | 1:A:35:ALA:HB1 | 2:B:126:ILE:HD13 | 2 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 4 | 0.6 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 4 | 0.6 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 4 | 0.6 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 3 | 0.6 |
| (2,3175) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 3 | 0.6 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 6 | 0.6 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 6 | 0.6 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 6 | 0.6 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 6 | 0.6 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 6 | 0.6 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 6 | 0.6 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 3 | 0.6 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 3 | 0.6 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 3 | 0.6 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 3 | 0.6 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 3 | 0.6 |
| (2,2580) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 5 | 0.6 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 5 | 0.6 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 5 | 0.6 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 5 | 0.6 |
| (2,2256) | 1:A:25:GLU:HG3 | 1:A:29:ASN:HD22 | 2 | 0.6 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD21 | 2 | 0.6 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD22 | 2 | 0.6 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 1 | 0.6 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 1 | 0.6 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 1 | 0.6 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 1 | 0.6 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 1 | 0.6 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 1 | 0.6 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 1 | 0.6 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 1 | 0.6 |
| (2,1238) | 2:B:165:VAL:HA | 2:B:165:VAL:HG12 | 7 | 0.6 |
| (2,1238) | 2:B:165:VAL:HA | 2:B:165:VAL:HG11 | 7 | 0.6 |
| (2,1238) | 2:B:165:VAL:HA | 2:B:165:VAL:HG13 | 7 | 0.6 |
| (2,1238) | 2:B:165:VAL:HA | 2:B:165:VAL:HG22 | 7 | 0.6 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 6 | 0.6 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 6 | 0.6 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 6 | 0.59 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 6 | 0.59 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 6 | 0.59 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 9 | 0.59 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 9 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 9 | 0.59 |
| (2,795) | 2:B:104:VAL:HG12 | 2:B:103:TYR:HA | 8 | 0.59 |
| (2,795) | 2:B:104:VAL:HG11 | 2:B:103:TYR:HA | 8 | 0.59 |
| (2,795) | 2:B:104:VAL:HG13 | 2:B:103:TYR:HA | 8 | 0.59 |
| (2,795) | 2:B:104:VAL:HG22 | 2:B:103:TYR:HA | 8 | 0.59 |
| (2,795) | 2:B:104:VAL:HG12 | 2:B:103:TYR:HA | 10 | 0.59 |
| (2,795) | 2:B:104:VAL:HG11 | 2:B:103:TYR:HA | 10 | 0.59 |
| (2,795) | 2:B:104:VAL:HG13 | 2:B:103:TYR:HA | 10 | 0.59 |
| (2,795) | 2:B:104:VAL:HG22 | 2:B:103:TYR:HA | 10 | 0.59 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 4 | 0.59 |
| (2,4462) | 2:B:125:LYS:H | 2:B:125:LYS:HB2 | 5 | 0.59 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 2 | 0.59 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 5 | 0.59 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 2 | 0.59 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 2 | 0.59 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 7 | 0.59 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 7 | 0.59 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.59 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.59 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.59 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 3 | 0.59 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 3 | 0.59 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 3 | 0.59 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 6 | 0.59 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 6 | 0.59 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 6 | 0.59 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 9 | 0.59 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 9 | 0.59 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 9 | 0.59 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 7 | 0.59 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 7 | 0.59 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 7 | 0.59 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 4 | 0.59 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 4 | 0.59 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 4 | 0.59 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 4 | 0.59 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 1 | 0.59 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 1 | 0.59 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 1 | 0.59 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 5 | 0.59 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 5 | 0.59 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 5 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 6 | 0.59 |
| (2,1374) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 6 | 0.59 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 5 | 0.58 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 5 | 0.58 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 5 | 0.58 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 5 | 0.58 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 5 | 0.58 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 8 | 0.58 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 8 | 0.58 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 8 | 0.58 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 8 | 0.58 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 8 | 0.58 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 10 | 0.58 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 10 | 0.58 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 10 | 0.58 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 10 | 0.58 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 10 | 0.58 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 1 | 0.58 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 1 | 0.58 |
| (2,752) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 1 | 0.58 |
| (2,752) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 1 | 0.58 |
| (2,4291) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 3 | 0.58 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 2 | 0.58 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 10 | 0.58 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 0.58 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 10 | 0.58 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 10 | 0.58 |
| (2,3221) | 2:B:159:ILE:HD12 | 2:B:158:GLY:H | 4 | 0.58 |
| (2,3221) | 2:B:159:ILE:HD13 | 2:B:158:GLY:H | 4 | 0.58 |
| (2,3221) | 2:B:159:ILE:HD12 | 1:A:61:CYS:H | 4 | 0.58 |
| (2,3221) | 2:B:159:ILE:HD13 | 1:A:61:CYS:H | 4 | 0.58 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 4 | 0.58 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 4 | 0.58 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 4 | 0.58 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 4 | 0.58 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 3 | 0.58 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 3 | 0.58 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 5 | 0.58 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 5 | 0.58 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD12 | 10 | 0.58 |
| (2,2771) | 2:B:116:SER:HA | 2:B:151:ILE:HD11 | 10 | 0.58 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 7 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 7 | 0.58 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 7 | 0.58 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 7 | 0.58 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 7 | 0.58 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 8 | 0.58 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 8 | 0.58 |
| (2,2626) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 8 | 0.58 |
| (2,2626) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 8 | 0.58 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 8 | 0.58 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 8 | 0.58 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 8 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 1 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 1 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 1 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 4 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 4 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 4 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 8 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 8 | 0.58 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 8 | 0.58 |
| (2,2013) | 2:B:165:VAL:HA | 2:B:165:VAL:HG12 | 7 | 0.58 |
| (2,2013) | 2:B:165:VAL:HA | 2:B:165:VAL:HG11 | 7 | 0.58 |
| (2,2013) | 2:B:165:VAL:HA | 2:B:165:VAL:HG13 | 7 | 0.58 |
| (2,2013) | 2:B:165:VAL:HA | 2:B:165:VAL:HG22 | 7 | 0.58 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 2 | 0.58 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 2 | 0.58 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 2 | 0.58 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 7 | 0.58 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 7 | 0.58 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 7 | 0.58 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 10 | 0.58 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 10 | 0.58 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 10 | 0.58 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 10 | 0.58 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 4 | 0.57 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 4 | 0.57 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 4 | 0.57 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 4 | 0.57 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 4 | 0.57 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 4 | 0.57 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 4 | 0.57 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 1 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4291) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 6 | 0.57 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 4 | 0.57 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 4 | 0.57 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 4 | 0.57 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 1 | 0.57 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 1 | 0.57 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 2 | 0.57 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 2 | 0.57 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 2 | 0.57 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 2 | 0.57 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 2 | 0.57 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 2 | 0.57 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 7 | 0.57 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 7 | 0.57 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 7 | 0.57 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 7 | 0.57 |
| (2,2703) | 2:B:109:LEU:HD12 | 2:B:109:LEU:H | 4 | 0.57 |
| (2,2703) | 2:B:109:LEU:HD13 | 2:B:109:LEU:H | 4 | 0.57 |
| (2,2703) | 2:B:109:LEU:HD22 | 2:B:109:LEU:H | 4 | 0.57 |
| (2,2703) | 2:B:109:LEU:HD21 | 2:B:109:LEU:H | 4 | 0.57 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 4 | 0.57 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 4 | 0.57 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 4 | 0.57 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 2 | 0.57 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 2 | 0.57 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 2 | 0.57 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 7 | 0.57 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 7 | 0.57 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 7 | 0.57 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 3 | 0.57 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 3 | 0.57 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 3 | 0.57 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 9 | 0.57 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 9 | 0.57 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 9 | 0.57 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 7 | 0.57 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 7 | 0.57 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 7 | 0.57 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.56 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.56 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.56 |
| (2,4458) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 1 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4458) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 2 | 0.56 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 3 | 0.56 |
| (2,4291) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 7 | 0.56 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 7 | 0.56 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 10 | 0.56 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 5 | 0.56 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 6 | 0.56 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 8 | 0.56 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 10 | 0.56 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 7 | 0.56 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 10 | 0.56 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 3 | 0.56 |
| (2,3857) | 2:B:125:LYS:H | 2:B:125:LYS:HE3 | 10 | 0.56 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 6 | 0.56 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 6 | 0.56 |
| (2,3440) | 1:A:8:ALA:HA | 2:B:109:LEU:HD12 | 4 | 0.56 |
| (2,3440) | 1:A:8:ALA:HA | 2:B:109:LEU:HD13 | 4 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 10 | 0.56 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 10 | 0.56 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.56 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.56 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.56 |
| (2,2580) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 7 | 0.56 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 7 | 0.56 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 7 | 0.56 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 7 | 0.56 |
| (2,2256) | 1:A:25:GLU:HG3 | 1:A:29:ASN:HD22 | 5 | 0.56 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD21 | 5 | 0.56 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD22 | 5 | 0.56 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 3 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 3 | 0.56 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 5 | 0.56 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 5 | 0.56 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 9 | 0.56 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 9 | 0.56 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 9 | 0.56 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 9 | 0.56 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 6 | 0.56 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 6 | 0.56 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 6 | 0.56 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 6 | 0.56 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 10 | 0.56 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 10 | 0.56 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 5 | 0.55 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 5 | 0.55 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 5 | 0.55 |
| (2,693) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD1 | 6 | 0.55 |
| (2,693) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD2 | 6 | 0.55 |
| (2,693) | 1:A:51:LEU:HD11 | 1:A:47:PHE:HD1 | 6 | 0.55 |
| (2,693) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD1 | 6 | 0.55 |
| (2,693) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD2 | 6 | 0.55 |
| (2,4290) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 3 | 0.55 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 7 | 0.55 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 3 | 0.55 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 4 | 0.55 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 1 | 0.55 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 1 | 0.55 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 1 | 0.55 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 4 | 0.55 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 4 | 0.55 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 4 | 0.55 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 8 | 0.55 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 8 | 0.55 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 8 | 0.55 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 5 | 0.55 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 5 | 0.55 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 5 | 0.55 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 8 | 0.55 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 8 | 0.55 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 8 | 0.55 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 8 | 0.55 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 5 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 5 | 0.55 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 5 | 0.55 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 7 | 0.55 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 7 | 0.55 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 3 | 0.55 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 3 | 0.55 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 3 | 0.55 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 6 | 0.55 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 6 | 0.55 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 8 | 0.55 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 8 | 0.55 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 10 | 0.55 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 10 | 0.55 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 3 | 0.55 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 3 | 0.55 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 5 | 0.55 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 5 | 0.55 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 5 | 0.55 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 5 | 0.55 |
| (2,1032) | 2:B:134:ALA:HB2 | 2:B:124:LYS:HE2 | 6 | 0.55 |
| (2,1032) | 2:B:134:ALA:HB1 | 2:B:124:LYS:HE2 | 6 | 0.55 |
| (2,1032) | 2:B:134:ALA:HB3 | 2:B:124:LYS:HE2 | 6 | 0.55 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 3 | 0.54 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 3 | 0.54 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 3 | 0.54 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 3 | 0.54 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 3 | 0.54 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 2 | 0.54 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 2 | 0.54 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 2 | 0.54 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 9 | 0.54 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 9 | 0.54 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 9 | 0.54 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 9 | 0.54 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 9 | 0.54 |
| (2,4291) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 10 | 0.54 |
| (2,4290) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 6 | 0.54 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 9 | 0.54 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 2 | 0.54 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 5 | 0.54 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 5 | 0.54 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 6 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 8 | 0.54 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 10 | 0.54 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 2 | 0.54 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 9 | 0.54 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 9 | 0.54 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 2 | 0.54 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 2 | 0.54 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 2 | 0.54 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 7 | 0.54 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 7 | 0.54 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 7 | 0.54 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 8 | 0.54 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 8 | 0.54 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 8 | 0.54 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 9 | 0.54 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 9 | 0.54 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 9 | 0.54 |
| (2,3221) | 2:B:159:ILE:HD12 | 2:B:158:GLY:H | 7 | 0.54 |
| (2,3221) | 2:B:159:ILE:HD13 | 2:B:158:GLY:H | 7 | 0.54 |
| (2,3221) | 2:B:159:ILE:HD12 | 1:A:61:CYS:H | 7 | 0.54 |
| (2,3221) | 2:B:159:ILE:HD13 | 1:A:61:CYS:H | 7 | 0.54 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 2 | 0.54 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 2 | 0.54 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 2 | 0.54 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 2 | 0.54 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 5 | 0.54 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 5 | 0.54 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 6 | 0.54 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 6 | 0.54 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 5 | 0.54 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 5 | 0.54 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 5 | 0.54 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 5 | 0.54 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 7 | 0.54 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 7 | 0.54 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 7 | 0.54 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 7 | 0.54 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 2 | 0.54 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 2 | 0.54 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 2 | 0.54 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 2 | 0.54 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 2 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 2 | 0.54 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 2 | 0.54 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 5 | 0.54 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 5 | 0.54 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 5 | 0.54 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 2 | 0.54 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 2 | 0.54 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 6 | 0.54 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 6 | 0.54 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 8 | 0.54 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 8 | 0.54 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 10 | 0.54 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 10 | 0.54 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 9 | 0.54 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 9 | 0.54 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 9 | 0.54 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 10 | 0.54 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 10 | 0.54 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 10 | 0.54 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 2 | 0.54 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 2 | 0.54 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 2 | 0.54 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 2 | 0.54 |
| (2,1486) | 1:A:39:VAL:HG12 | 1:A:5:SER:HA | 7 | 0.54 |
| (2,1486) | 1:A:39:VAL:HG11 | 1:A:5:SER:HA | 7 | 0.54 |
| (2,1486) | 1:A:39:VAL:HG13 | 1:A:5:SER:HA | 7 | 0.54 |
| (2,1486) | 1:A:39:VAL:HG22 | 1:A:5:SER:HA | 7 | 0.54 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 2 | 0.53 |
| (2,4290) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 7 | 0.53 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 10 | 0.53 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 2 | 0.53 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 3 | 0.53 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 2 | 0.53 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 1 | 0.53 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 1 | 0.53 |
| (2,3431) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 9 | 0.53 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 9 | 0.53 |
| (2,3431) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 9 | 0.53 |
| (2,3390) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 3 | 0.53 |
| (2,3390) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 3 | 0.53 |
| (2,3390) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 3 | 0.53 |
| (2,3390) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 3 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3390) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 3 | 0.53 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 7 | 0.53 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 7 | 0.53 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 7 | 0.53 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 7 | 0.53 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 7 | 0.53 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 7 | 0.53 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 7 | 0.53 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD21 | 9 | 0.53 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD22 | 9 | 0.53 |
| (2,2579) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HD21 | 9 | 0.53 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 8 | 0.53 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 8 | 0.53 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 8 | 0.53 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 8 | 0.53 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 9 | 0.53 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 9 | 0.53 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 9 | 0.53 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 2 | 0.53 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 2 | 0.53 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 5 | 0.53 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 5 | 0.53 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 5 | 0.53 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 1 | 0.53 |
| (2,1620) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 1 | 0.53 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 10 | 0.53 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 10 | 0.53 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 10 | 0.53 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 10 | 0.53 |
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 2 | 0.53 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 2 | 0.53 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 2 | 0.53 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 2 | 0.53 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 7 | 0.52 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 7 | 0.52 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 7 | 0.52 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 7 | 0.52 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 7 | 0.52 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 1 | 0.52 |
| (2,4521) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 6 | 0.52 |
| (2,4458) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 10 | 0.52 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 9 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 8 | 0.52 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 2 | 0.52 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 4 | 0.52 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 7 | 0.52 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 8 | 0.52 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 9 | 0.52 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 3 | 0.52 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 3 | 0.52 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 8 | 0.52 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 8 | 0.52 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 3 | 0.52 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 3 | 0.52 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 3 | 0.52 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 5 | 0.52 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 5 | 0.52 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 5 | 0.52 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 5 | 0.52 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 4 | 0.52 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 4 | 0.52 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 4 | 0.52 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 2 | 0.52 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 2 | 0.52 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 5 | 0.52 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 5 | 0.52 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 5 | 0.52 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 5 | 0.52 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 1 | 0.52 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 1 | 0.52 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 8 | 0.52 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 8 | 0.52 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 5 | 0.52 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 5 | 0.52 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 5 | 0.52 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 4 | 0.52 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 4 | 0.52 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG22 | 8 | 0.52 |
| (2,1945) | 2:B:149:LYS:HB3 | 2:B:154:VAL:HG22 | 8 | 0.52 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG21 | 8 | 0.52 |
| (2,1945) | 2:B:149:LYS:HB3 | 2:B:154:VAL:HG21 | 8 | 0.52 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG23 | 8 | 0.52 |
| (2,1809) | 2:B:132:ILE:HG22 | 1:A:18:ASP:HB2 | 5 | 0.52 |
| (2,1809) | 2:B:132:ILE:HG23 | 1:A:18:ASP:HB2 | 5 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 2 | 0.52 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 2 | 0.52 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 2 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 3 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 3 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 3 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 3 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 3 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 3 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 3 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 3 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 5 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 5 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 5 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 5 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 5 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 5 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 5 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 5 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 6 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 6 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 6 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 6 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 6 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 6 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 6 | 0.52 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 6 | 0.52 |
| (2,792) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 8 | 0.51 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 8 | 0.51 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 8 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 8 | 0.51 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 8 | 0.51 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 10 | 0.51 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 10 | 0.51 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 10 | 0.51 |
| (2,754) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 10 | 0.51 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 1 | 0.51 |
| (2,4290) | 1:A:26:ASP:HB3 | 1:A:26:ASP:H | 10 | 0.51 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 9 | 0.51 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 2 | 0.51 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 6 | 0.51 |
| (2,384) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 6 | 0.51 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 3 | 0.51 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 7 | 0.51 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 5 | 0.51 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 5 | 0.51 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 5 | 0.51 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 4 | 0.51 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 4 | 0.51 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 1 | 0.51 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 1 | 0.51 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 1 | 0.51 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 1 | 0.51 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 2 | 0.51 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 2 | 0.51 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 2 | 0.51 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 2 | 0.51 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 2 | 0.51 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 2 | 0.51 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 2 | 0.51 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 1 | 0.51 |
| (2,2640) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 1 | 0.51 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 8 | 0.51 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 8 | 0.51 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 8 | 0.51 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 2 | 0.51 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 2 | 0.51 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 2 | 0.51 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 2 | 0.51 |
| (2,2023) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 0.51 |
| (2,2023) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 0.51 |
| (2,2023) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2023) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 0.51 |
| (2,2023) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 0.51 |
| (2,2023) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 0.51 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 4 | 0.51 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 4 | 0.51 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 8 | 0.51 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 8 | 0.51 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 8 | 0.51 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 8 | 0.51 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 8 | 0.51 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 1 | 0.5 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 1 | 0.5 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 1 | 0.5 |
| (2,760) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 9 | 0.5 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 9 | 0.5 |
| (2,760) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 9 | 0.5 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 3 | 0.5 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 3 | 0.5 |
| (2,4520) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 8 | 0.5 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 7 | 0.5 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 6 | 0.5 |
| (2,4080) | 2:B:122:ASP:HA | 2:B:125:LYS:HB2 | 10 | 0.5 |
| (2,3836) | 2:B:122:ASP:H | 2:B:121:LYS:HB3 | 10 | 0.5 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 9 | 0.5 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 9 | 0.5 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 9 | 0.5 |
| (2,3513) | 2:B:155:ILE:HG22 | 1:A:11:TYR:HE2 | 1 | 0.5 |
| (2,3513) | 2:B:155:ILE:HG21 | 1:A:11:TYR:HE2 | 1 | 0.5 |
| (2,3513) | 2:B:155:ILE:HG23 | 1:A:11:TYR:HE2 | 1 | 0.5 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 1 | 0.5 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 1 | 0.5 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 1 | 0.5 |
| (2,3145) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 7 | 0.5 |
| (2,3145) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 7 | 0.5 |
| (2,3145) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 7 | 0.5 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 6 | 0.5 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 6 | 0.5 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 6 | 0.5 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 6 | 0.5 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 5 | 0.5 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 5 | 0.5 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 5 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 5 | 0.5 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 5 | 0.5 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 5 | 0.5 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 5 | 0.5 |
| (2,3017) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 3 | 0.5 |
| (2,3017) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 3 | 0.5 |
| (2,3017) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 3 | 0.5 |
| (2,3017) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 3 | 0.5 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 6 | 0.5 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 6 | 0.5 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 6 | 0.5 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 6 | 0.5 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 6 | 0.5 |
| (2,2600) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 9 | 0.5 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 9 | 0.5 |
| (2,2600) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 9 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 7 | 0.5 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 7 | 0.5 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 7 | 0.5 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 7 | 0.5 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 7 | 0.5 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 8 | 0.49 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 8 | 0.49 |
| (2,4521) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 5 | 0.49 |
| (2,4462) | 2:B:125:LYS:H | 2:B:125:LYS:HB2 | 10 | 0.49 |
| (2,4458) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 5 | 0.49 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 4 | 0.49 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 5 | 0.49 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 6 | 0.49 |
| (2,4201) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 1 | 0.49 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 1 | 0.49 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 3 | 0.49 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 1 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD11 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD13 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD12 | 2:B:108:LEU:HB2 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD11 | 2:B:108:LEU:HB2 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD13 | 2:B:108:LEU:HB2 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD22 | 2:B:109:LEU:HD12 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD22 | 2:B:109:LEU:HD13 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD21 | 2:B:109:LEU:HD12 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD21 | 2:B:109:LEU:HD13 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 6 | 0.49 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 6 | 0.49 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD12 | 6 | 0.49 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 1 | 0.49 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 1 | 0.49 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 1 | 0.49 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 10 | 0.49 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 10 | 0.49 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 10 | 0.49 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 10 | 0.49 |
| (2,2494) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD2 | 6 | 0.49 |
| (2,2494) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD1 | 6 | 0.49 |
| (2,2494) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD2 | 6 | 0.49 |
| (2,2494) | 1:A:51:LEU:HD11 | 1:A:47:PHE:HD1 | 6 | 0.49 |
| (2,2494) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD1 | 6 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 3 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 3 | 0.49 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 3 | 0.49 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD11 | 6 | 0.48 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD13 | 6 | 0.48 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD11 | 6 | 0.48 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD13 | 6 | 0.48 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 10 | 0.48 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 10 | 0.48 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 6 | 0.48 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 8 | 0.48 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 10 | 0.48 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 7 | 0.48 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 4 | 0.48 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 10 | 0.48 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 10 | 0.48 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 5 | 0.48 |
| (2,4124) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 5 | 0.48 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 7 | 0.48 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 5 | 0.48 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 7 | 0.48 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 4 | 0.48 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 10 | 0.48 |
| (2,3430) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 3 | 0.48 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 3 | 0.48 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 3 | 0.48 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 10 | 0.48 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 10 | 0.48 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 9 | 0.48 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 9 | 0.48 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 9 | 0.48 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 9 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 5 | 0.48 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 5 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 10 | 0.48 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 10 | 0.48 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 10 | 0.48 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 10 | 0.48 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 4 | 0.48 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 4 | 0.48 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 4 | 0.48 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 4 | 0.48 |
| (2,950) | 2:B:125:LYS:HB2 | 2:B:122:ASP:HB2 | 10 | 0.47 |
| (2,950) | 2:B:125:LYS:HB2 | 2:B:122:ASP:HB3 | 10 | 0.47 |
| (2,795) | 2:B:104:VAL:HG12 | 2:B:103:TYR:HA | 7 | 0.47 |
| (2,795) | 2:B:104:VAL:HG11 | 2:B:103:TYR:HA | 7 | 0.47 |
| (2,795) | 2:B:104:VAL:HG13 | 2:B:103:TYR:HA | 7 | 0.47 |
| (2,795) | 2:B:104:VAL:HG22 | 2:B:103:TYR:HA | 7 | 0.47 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 2 | 0.47 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 2 | 0.47 |
| (2,4562) | 2:B:163:ALA:HA | 2:B:163:ALA:H | 9 | 0.47 |
| (2,4521) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 3 | 0.47 |
| (2,4521) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 7 | 0.47 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 2 | 0.47 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 9 | 0.47 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 1 | 0.47 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 2 | 0.47 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 3 | 0.47 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 4 | 0.47 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 5 | 0.47 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 8 | 0.47 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 9 | 0.47 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 10 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 5 | 0.47 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 2 | 0.47 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 4 | 0.47 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 7 | 0.47 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 8 | 0.47 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 9 | 0.47 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 4 | 0.47 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 5 | 0.47 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 5 | 0.47 |
| (2,3205) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 8 | 0.47 |
| (2,3205) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 8 | 0.47 |
| (2,3205) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 8 | 0.47 |
| (2,3205) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 8 | 0.47 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 2 | 0.47 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 2 | 0.47 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 2 | 0.47 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 2 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 10 | 0.47 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 10 | 0.47 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 5 | 0.47 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 5 | 0.47 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 2 | 0.47 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 2 | 0.47 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 2 | 0.47 |
| (2,2069) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 6 | 0.47 |
| (2,2069) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 6 | 0.47 |
| (2,2069) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 6 | 0.47 |
| (2,1654) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 8 | 0.47 |
| (2,1654) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 8 | 0.47 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 8 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 8 | 0.47 |
| (2,951) | 2:B:125:LYS:HD2 | 2:B:129:SER:HB3 | 3 | 0.46 |
| (2,951) | 2:B:125:LYS:HD3 | 2:B:129:SER:HB3 | 3 | 0.46 |
| (2,795) | 2:B:104:VAL:HG12 | 2:B:103:TYR:HA | 6 | 0.46 |
| (2,795) | 2:B:104:VAL:HG11 | 2:B:103:TYR:HA | 6 | 0.46 |
| (2,795) | 2:B:104:VAL:HG13 | 2:B:103:TYR:HA | 6 | 0.46 |
| (2,795) | 2:B:104:VAL:HG22 | 2:B:103:TYR:HA | 6 | 0.46 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD11 | 10 | 0.46 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD13 | 10 | 0.46 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD11 | 10 | 0.46 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD13 | 10 | 0.46 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 9 | 0.46 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 9 | 0.46 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 9 | 0.46 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 9 | 0.46 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 1 | 0.46 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 1 | 0.46 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 7 | 0.46 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 7 | 0.46 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 2 | 0.46 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 10 | 0.46 |
| (2,4410) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 3 | 0.46 |
| (2,4376) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 6 | 0.46 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 9 | 0.46 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 1 | 0.46 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 5 | 0.46 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 3 | 0.46 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 7 | 0.46 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 3 | 0.46 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 6 | 0.46 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 8 | 0.46 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 10 | 0.46 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 3 | 0.46 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 3 | 0.46 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 3 | 0.46 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 3 | 0.46 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 1 | 0.46 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 1 | 0.46 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 7 | 0.46 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 7 | 0.46 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 9 | 0.46 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 9 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 9 | 0.46 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 9 | 0.46 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG22 | 6 | 0.46 |
| (2,1945) | 2:B:149:LYS:HB3 | 2:B:154:VAL:HG22 | 6 | 0.46 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG21 | 6 | 0.46 |
| (2,1945) | 2:B:149:LYS:HB3 | 2:B:154:VAL:HG21 | 6 | 0.46 |
| (2,1945) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG23 | 6 | 0.46 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 6 | 0.46 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 6 | 0.46 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 6 | 0.46 |
| (2,1540) | 1:A:47:PHE:HA | 1:A:51:LEU:HD12 | 7 | 0.46 |
| (2,1540) | 1:A:47:PHE:HA | 1:A:51:LEU:HD13 | 7 | 0.46 |
| (2,1540) | 1:A:56:ILE:HA | 1:A:51:LEU:HD13 | 7 | 0.46 |
| (2,1540) | 1:A:56:ILE:HA | 1:A:51:LEU:HD23 | 7 | 0.46 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 5 | 0.46 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 5 | 0.46 |
| (2,795) | 2:B:104:VAL:HG12 | 2:B:103:TYR:HA | 4 | 0.45 |
| (2,795) | 2:B:104:VAL:HG11 | 2:B:103:TYR:HA | 4 | 0.45 |
| (2,795) | 2:B:104:VAL:HG13 | 2:B:103:TYR:HA | 4 | 0.45 |
| (2,795) | 2:B:104:VAL:HG22 | 2:B:103:TYR:HA | 4 | 0.45 |
| (2,795) | 2:B:104:VAL:HG12 | 2:B:103:TYR:HA | 9 | 0.45 |
| (2,795) | 2:B:104:VAL:HG11 | 2:B:103:TYR:HA | 9 | 0.45 |
| (2,795) | 2:B:104:VAL:HG13 | 2:B:103:TYR:HA | 9 | 0.45 |
| (2,795) | 2:B:104:VAL:HG22 | 2:B:103:TYR:HA | 9 | 0.45 |
| (2,522) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 8 | 0.45 |
| (2,522) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 8 | 0.45 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 6 | 0.45 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 2 | 0.45 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 4 | 0.45 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 7 | 0.45 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 8 | 0.45 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 10 | 0.45 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 9 | 0.45 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 2 | 0.45 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 9 | 0.45 |
| (2,3841) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 1 | 0.45 |
| (2,3841) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 5 | 0.45 |
| (2,3841) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 8 | 0.45 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 4 | 0.45 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 4 | 0.45 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 4 | 0.45 |
| (2,2286) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 8 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2286) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 8 | 0.45 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 9 | 0.45 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 9 | 0.45 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 9 | 0.45 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 9 | 0.45 |
| (2,1510) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 8 | 0.45 |
| (2,1510) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 8 | 0.45 |
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 3 | 0.45 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 3 | 0.45 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 3 | 0.45 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 3 | 0.45 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 1 | 0.45 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 1 | 0.45 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 1 | 0.45 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 1 | 0.45 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 1 | 0.44 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 1 | 0.44 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 1 | 0.44 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 6 | 0.44 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 6 | 0.44 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 6 | 0.44 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 6 | 0.44 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 6 | 0.44 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 3 | 0.44 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 8 | 0.44 |
| (2,421) | 1:A:15:ILE:HD11 | 2:B:106:SER:HA | 4 | 0.44 |
| (2,421) | 1:A:15:ILE:HD13 | 2:B:106:SER:HA | 4 | 0.44 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 1 | 0.44 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 3 | 0.44 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 3 | 0.44 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 3 | 0.44 |
| (2,4067) | 1:A:11:TYR:HA | 1:A:11:TYR:HD2 | 3 | 0.44 |
| (2,3841) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 2 | 0.44 |
| (2,3841) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 3 | 0.44 |
| (2,370) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 6 | 0.44 |
| (2,370) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 6 | 0.44 |
| (2,370) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 6 | 0.44 |
| (2,3430) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 1 | 0.44 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 1 | 0.44 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 1 | 0.44 |
| (2,3142) | 2:B:151:ILE:HD12 | 2:B:150:ASN:HA | 8 | 0.44 |
| (2,3142) | 2:B:151:ILE:HD13 | 2:B:150:ASN:HA | 8 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD12 | 2 | 0.44 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD11 | 2 | 0.44 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD13 | 2 | 0.44 |
| (2,3113) | 2:B:146:LEU:H | 2:B:146:LEU:HD22 | 2 | 0.44 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 5 | 0.44 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 5 | 0.44 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 5 | 0.44 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 5 | 0.44 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 7 | 0.44 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 7 | 0.44 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 7 | 0.44 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 7 | 0.44 |
| (2,3096) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 9 | 0.44 |
| (2,3096) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 9 | 0.44 |
| (2,3096) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 9 | 0.44 |
| (2,3096) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 9 | 0.44 |
| (2,3017) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 2 | 0.44 |
| (2,3017) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 2 | 0.44 |
| (2,3017) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 2 | 0.44 |
| (2,3017) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 2 | 0.44 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB2 | 9 | 0.44 |
| (2,3006) | 2:B:138:ARG:HD2 | 2:B:137:ASP:HB3 | 9 | 0.44 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 1 | 0.44 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 1 | 0.44 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 1 | 0.44 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.44 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.44 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.44 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 9 | 0.44 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 9 | 0.44 |
| (2,2626) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 9 | 0.44 |
| (2,2626) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 9 | 0.44 |
| (2,2580) | 1:A:61:CYS:HB2 | 1:A:60:ILE:HG21 | 1 | 0.44 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG22 | 1 | 0.44 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG21 | 1 | 0.44 |
| (2,2580) | 1:A:61:CYS:HB3 | 1:A:60:ILE:HG23 | 1 | 0.44 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 1 | 0.44 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 1 | 0.44 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 1 | 0.44 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 1 | 0.44 |
| (2,1878) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD12 | 4 | 0.44 |
| (2,1878) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD11 | 4 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1878) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD13 | 4 | 0.44 |
| (2,1878) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD12 | 4 | 0.44 |
| (2,1878) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD13 | 4 | 0.44 |
| (2,1809) | 2:B:132:ILE:HG22 | 1:A:18:ASP:HB2 | 8 | 0.44 |
| (2,1809) | 2:B:132:ILE:HG23 | 1:A:18:ASP:HB2 | 8 | 0.44 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 3 | 0.44 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 3 | 0.44 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 3 | 0.44 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 4 | 0.44 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 4 | 0.44 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 4 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 2 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 2 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 2 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 2 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 2 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 2 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 2 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 2 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 7 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 7 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 7 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 7 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 7 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 7 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 7 | 0.44 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 7 | 0.44 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 4 | 0.44 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 4 | 0.44 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 4 | 0.44 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 4 | 0.44 |
| (2,1059) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 3 | 0.44 |
| (2,1059) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 3 | 0.44 |
| (2,1059) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 3 | 0.44 |
| (2,1059) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 3 | 0.44 |
| (2,826) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 3 | 0.43 |
| (2,826) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 3 | 0.43 |
| (2,826) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 3 | 0.43 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 4 | 0.43 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 4 | 0.43 |
| (2,4206) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 5 | 0.43 |
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 6 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4197) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 9 | 0.43 |
| (2,4141) | 1:A:27:LYS:HA | 1:A:27:LYS:HD2 | 9 | 0.43 |
| (2,3858) | 2:B:125:LYS:H | 2:B:125:LYS:HB2 | 5 | 0.43 |
| (2,3841) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 6 | 0.43 |
| (2,3841) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 10 | 0.43 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 8 | 0.43 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 8 | 0.43 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 8 | 0.43 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 8 | 0.43 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 9 | 0.43 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 9 | 0.43 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 9 | 0.43 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 9 | 0.43 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 4 | 0.43 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 4 | 0.43 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 4 | 0.43 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 4 | 0.43 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD12 | 10 | 0.43 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD13 | 10 | 0.43 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD22 | 10 | 0.43 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 10 | 0.43 |
| (2,1136) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB2 | 10 | 0.43 |
| (2,1136) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB3 | 10 | 0.43 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 10 | 0.43 |
| (2,940) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 8 | 0.42 |
| (2,940) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 8 | 0.42 |
| (2,940) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 8 | 0.42 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.42 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.42 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.42 |
| (2,621) | 1:A:40:GLU:HG2 | 1:A:42:PHE:HE2 | 6 | 0.42 |
| (2,621) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE1 | 6 | 0.42 |
| (2,621) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE2 | 6 | 0.42 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD11 | 7 | 0.42 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD13 | 7 | 0.42 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD11 | 7 | 0.42 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD13 | 7 | 0.42 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 7 | 0.42 |
| (2,4172) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 8 | 0.42 |
| (2,4118) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 1 | 0.42 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 4 | 0.42 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 1 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 5 | 0.42 |
| (2,4069) | 2:B:105:ALA:HA | 2:B:108:LEU:HB3 | 8 | 0.42 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 7 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG22 | 2:B:109:LEU:HD12 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG22 | 2:B:109:LEU:HD11 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG22 | 2:B:109:LEU:HD13 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG22 | 2:B:112:LEU:HD22 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG22 | 2:B:112:LEU:HD21 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG22 | 2:B:112:LEU:HD23 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG21 | 2:B:109:LEU:HD12 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG21 | 2:B:109:LEU:HD11 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG21 | 2:B:109:LEU:HD13 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG21 | 2:B:112:LEU:HD22 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG21 | 2:B:112:LEU:HD21 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG21 | 2:B:112:LEU:HD23 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG23 | 2:B:109:LEU:HD12 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG23 | 2:B:109:LEU:HD11 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG23 | 2:B:109:LEU:HD13 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG23 | 2:B:112:LEU:HD22 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG23 | 2:B:112:LEU:HD21 | 4 | 0.42 |
| (2,3395) | 1:A:39:VAL:HG23 | 2:B:112:LEU:HD23 | 4 | 0.42 |
| (2,3390) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 1 | 0.42 |
| (2,3390) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 1 | 0.42 |
| (2,3390) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 1 | 0.42 |
| (2,3390) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 1 | 0.42 |
| (2,3390) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 1 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 6 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 6 | 0.42 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 6 | 0.42 |
| (2,2852) | 2:B:123:ILE:HG22 | 2:B:103:TYR:HE2 | 8 | 0.42 |
| (2,2852) | 2:B:123:ILE:HG21 | 2:B:103:TYR:HE2 | 8 | 0.42 |
| (2,2852) | 2:B:123:ILE:HG23 | 2:B:103:TYR:HE2 | 8 | 0.42 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 2 | 0.42 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 2 | 0.42 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 2 | 0.42 |
| (2,2410) | 1:A:40:GLU:HG2 | 1:A:42:PHE:HE2 | 6 | 0.42 |
| (2,2410) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE1 | 6 | 0.42 |
| (2,2410) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE2 | 6 | 0.42 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 1 | 0.42 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 1 | 0.42 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 10 | 0.42 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 10 | 0.42 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 10 | 0.42 |
| (2,1608) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 10 | 0.42 |
| (2,1393) | 1:A:24:THR:HG21 | 1:A:26:ASP:HB3 | 3 | 0.42 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB2 | 3 | 0.42 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB3 | 3 | 0.42 |
| (2,1393) | 1:A:24:THR:HG23 | 1:A:26:ASP:HB3 | 3 | 0.42 |
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 9 | 0.42 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 9 | 0.42 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 9 | 0.42 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 9 | 0.42 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 7 | 0.41 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 4 | 0.41 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 2 | 0.41 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 4 | 0.41 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 7 | 0.41 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 8 | 0.41 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 10 | 0.41 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 1 | 0.41 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 1 | 0.41 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 1 | 0.41 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 1 | 0.41 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.41 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.41 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.41 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 4 | 0.41 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 4 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 4 | 0.41 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 4 | 0.41 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 1 | 0.41 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 1 | 0.41 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 1 | 0.41 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 1 | 0.41 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 1 | 0.41 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 8 | 0.41 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 8 | 0.41 |
| (2,1804) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 8 | 0.41 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 8 | 0.41 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 8 | 0.41 |
| (2,1800) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 8 | 0.41 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD12 | 8 | 0.41 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD11 | 8 | 0.41 |
| (2,1794) | 2:B:130:VAL:HG23 | 2:B:132:ILE:HD13 | 8 | 0.41 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 10 | 0.41 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 10 | 0.41 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 10 | 0.41 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 10 | 0.41 |
| (2,4375) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 8 | 0.4 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 1 | 0.4 |
| (2,4117) | 2:B:155:ILE:HA | 2:B:155:ILE:HG12 | 1 | 0.4 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 3 | 0.4 |
| (2,4049) | 1:A:59:LEU:HB3 | 1:A:60:ILE:HB | 8 | 0.4 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 1 | 0.4 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 1 | 0.4 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 1 | 0.4 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 1 | 0.4 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 1 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 10 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 10 | 0.4 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 10 | 0.4 |
| (2,2729) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 1 | 0.4 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 1 | 0.4 |
| (2,2729) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 1 | 0.4 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 1 | 0.4 |
| (2,2729) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 1 | 0.4 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 9 | 0.4 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 9 | 0.4 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 9 | 0.4 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 9 | 0.4 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 4 | 0.4 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 4 | 0.4 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 4 | 0.4 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 7 | 0.4 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 7 | 0.4 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 7 | 0.4 |
| (2,1598) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 7 | 0.4 |
| (2,1598) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 7 | 0.4 |
| (2,1598) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 7 | 0.4 |
| (2,1598) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 7 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 4 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 4 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 4 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 4 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 4 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 4 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 4 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 4 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 9 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 9 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 9 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 9 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 9 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 9 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 9 | 0.4 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 9 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 1 | 0.4 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 1 | 0.4 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 1 | 0.4 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 1 | 0.4 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD11 | 1 | 0.39 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD13 | 1 | 0.39 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD11 | 1 | 0.39 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD13 | 1 | 0.39 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 6 | 0.39 |
| (2,468) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 6 | 0.39 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 7 | 0.39 |
| (2,4549) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 9 | 0.39 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 8 | 0.39 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 6 | 0.39 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 6 | 0.39 |
| (2,4110) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 9 | 0.39 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 10 | 0.39 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 10 | 0.39 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 10 | 0.39 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 4 | 0.39 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 4 | 0.39 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 4 | 0.39 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 8 | 0.39 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 8 | 0.39 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 8 | 0.39 |
| (2,2647) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 8 | 0.39 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 1 | 0.39 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 1 | 0.39 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG22 | 9 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG21 | 9 | 0.39 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG23 | 9 | 0.39 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG12 | 9 | 0.39 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG11 | 9 | 0.39 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG22 | 9 | 0.39 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG21 | 9 | 0.39 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG23 | 9 | 0.39 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 1 | 0.39 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 1 | 0.39 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 1 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 2 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 2 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 2 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 3 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 3 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 3 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 8 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 8 | 0.39 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 8 | 0.39 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 9 | 0.39 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 9 | 0.39 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 9 | 0.39 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 9 | 0.39 |
| (2,795) | 2:B:104:VAL:HG12 | 2:B:103:TYR:HA | 1 | 0.38 |
| (2,795) | 2:B:104:VAL:HG11 | 2:B:103:TYR:HA | 1 | 0.38 |
| (2,795) | 2:B:104:VAL:HG13 | 2:B:103:TYR:HA | 1 | 0.38 |
| (2,795) | 2:B:104:VAL:HG22 | 2:B:103:TYR:HA | 1 | 0.38 |
| (2,621) | 1:A:40:GLU:HG2 | 1:A:42:PHE:HE2 | 4 | 0.38 |
| (2,621) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE1 | 4 | 0.38 |
| (2,621) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE2 | 4 | 0.38 |
| (2,4521) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 10 | 0.38 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 9 | 0.38 |
| (2,2681) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 9 | 0.38 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 9 | 0.38 |
| (2,2681) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 9 | 0.38 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 4 | 0.38 |
| (2,2626) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 4 | 0.38 |
| (2,2626) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 4 | 0.38 |
| (2,2626) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 4 | 0.38 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 10 | 0.38 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 10 | 0.38 |
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 10 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2591) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 10 | 0.38 |
| (2,2410) | 1:A:40:GLU:HG2 | 1:A:42:PHE:HE2 | 4 | 0.38 |
| (2,2410) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE1 | 4 | 0.38 |
| (2,2410) | 1:A:40:GLU:HG3 | 1:A:42:PHE:HE2 | 4 | 0.38 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 1 | 0.38 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 1 | 0.38 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 3 | 0.38 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 3 | 0.38 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 8 | 0.38 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 8 | 0.38 |
| (2,1765) | 2:B:126:ILE:HD12 | 2:B:125:LYS:HD2 | 4 | 0.38 |
| (2,1765) | 2:B:126:ILE:HD12 | 2:B:125:LYS:HD3 | 4 | 0.38 |
| (2,1765) | 2:B:126:ILE:HD11 | 2:B:125:LYS:HD2 | 4 | 0.38 |
| (2,1765) | 2:B:126:ILE:HD11 | 2:B:125:LYS:HD3 | 4 | 0.38 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 9 | 0.38 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 9 | 0.38 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 9 | 0.38 |
| (2,1059) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 2 | 0.38 |
| (2,1059) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 2 | 0.38 |
| (2,1059) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 2 | 0.38 |
| (2,1059) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 2 | 0.38 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 8 | 0.37 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 8 | 0.37 |
| (2,847) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 8 | 0.37 |
| (2,847) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 8 | 0.37 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 9 | 0.37 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 9 | 0.37 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 9 | 0.37 |
| (2,558) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 8 | 0.37 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 8 | 0.37 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 8 | 0.37 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD11 | 2 | 0.37 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD13 | 2 | 0.37 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD11 | 2 | 0.37 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD13 | 2 | 0.37 |
| (2,470) | 1:A:22:THR:HG21 | 1:A:27:LYS:HD3 | 5 | 0.37 |
| (2,470) | 1:A:22:THR:HG22 | 1:A:27:LYS:HD3 | 5 | 0.37 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD2 | 5 | 0.37 |
| (2,470) | 1:A:22:THR:HG23 | 1:A:27:LYS:HD3 | 5 | 0.37 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 10 | 0.37 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 2 | 0.37 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 10 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 9 | 0.37 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 2 | 0.37 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 2 | 0.37 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 2 | 0.37 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 2 | 0.37 |
| (2,2683) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 3 | 0.37 |
| (2,2683) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 3 | 0.37 |
| (2,2683) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 3 | 0.37 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 4 | 0.37 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 4 | 0.37 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 4 | 0.37 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 4 | 0.37 |
| (2,2257) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD21 | 2 | 0.37 |
| (2,2257) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD22 | 2 | 0.37 |
| (2,2257) | 1:A:25:GLU:HG3 | 1:A:29:ASN:HD22 | 2 | 0.37 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD11 | 6 | 0.37 |
| (2,2088) | 1:A:10:ILE:HB | 1:A:10:ILE:HD13 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD12 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD11 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD13 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD12 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD11 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD13 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD12 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD11 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD13 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD12 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD11 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD13 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD12 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD11 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD13 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD11 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD13 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD11 | 6 | 0.37 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD13 | 6 | 0.37 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 10 | 0.37 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 10 | 0.37 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 10 | 0.37 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 7 | 0.37 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 7 | 0.37 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 3 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 5 | 0.36 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 6 | 0.36 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 7 | 0.36 |
| (2,4120) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 9 | 0.36 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 7 | 0.36 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 7 | 0.36 |
| (2,3510) | 2:B:162:LEU:HD12 | 1:A:56:ILE:HG13 | 2 | 0.36 |
| (2,3510) | 2:B:162:LEU:HD11 | 1:A:56:ILE:HG13 | 2 | 0.36 |
| (2,3510) | 2:B:162:LEU:HD13 | 1:A:56:ILE:HG13 | 2 | 0.36 |
| (2,3510) | 2:B:162:LEU:HD21 | 1:A:56:ILE:HG13 | 2 | 0.36 |
| (2,3316) | 1:A:8:ALA:HB2 | 2:B:112:LEU:HD23 | 9 | 0.36 |
| (2,3316) | 1:A:8:ALA:HB1 | 2:B:112:LEU:HD22 | 9 | 0.36 |
| (2,3316) | 1:A:8:ALA:HB1 | 2:B:112:LEU:HD21 | 9 | 0.36 |
| (2,3316) | 1:A:8:ALA:HB1 | 2:B:112:LEU:HD23 | 9 | 0.36 |
| (2,3316) | 1:A:8:ALA:HB3 | 2:B:112:LEU:HD22 | 9 | 0.36 |
| (2,3316) | 1:A:8:ALA:HB3 | 2:B:112:LEU:HD23 | 9 | 0.36 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 1 | 0.36 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 1 | 0.36 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 1 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD11 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD13 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD12 | 2:B:108:LEU:HB2 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD11 | 2:B:108:LEU:HB2 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD13 | 2:B:108:LEU:HB2 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD22 | 2:B:109:LEU:HD12 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD22 | 2:B:109:LEU:HD13 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD21 | 2:B:109:LEU:HD12 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD21 | 2:B:109:LEU:HD13 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 10 | 0.36 |
| (2,2742) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 10 | 0.36 |
| (2,2742) | 2:B:112:LEU:HD23 | 2:B:109:LEU:HD12 | 10 | 0.36 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 9 | 0.36 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 9 | 0.36 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 9 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 9 | 0.36 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 9 | 0.36 |
| (2,2373) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 3 | 0.36 |
| (2,2373) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 3 | 0.36 |
| (2,2373) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 3 | 0.36 |
| (2,2373) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 3 | 0.36 |
| (2,2373) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 3 | 0.36 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 3 | 0.36 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 3 | 0.36 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 3 | 0.36 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 3 | 0.36 |
| (2,1654) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 6 | 0.36 |
| (2,1654) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 6 | 0.36 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 6 | 0.36 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 6 | 0.36 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG12 | 10 | 0.36 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG11 | 10 | 0.36 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG13 | 10 | 0.36 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG22 | 10 | 0.36 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG23 | 10 | 0.36 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 1 | 0.36 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 1 | 0.36 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 1 | 0.36 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 5 | 0.35 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 1 | 0.35 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 2 | 0.35 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 4 | 0.35 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 4 | 0.35 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 5 | 0.35 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 5 | 0.35 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 5 | 0.35 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 5 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 9 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 9 | 0.35 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 9 | 0.35 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 8 | 0.35 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 8 | 0.35 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 8 | 0.35 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 8 | 0.35 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 8 | 0.35 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 8 | 0.35 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 8 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD12 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD11 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD13 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD12 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD11 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD13 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD12 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD11 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD13 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD12 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD11 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD13 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD12 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD11 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD13 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD11 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD13 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD11 | 7 | 0.35 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD13 | 7 | 0.35 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 1 | 0.35 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 1 | 0.35 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 1 | 0.35 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG12 | 3 | 0.35 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG11 | 3 | 0.35 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG13 | 3 | 0.35 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG22 | 3 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG23 | 3 | 0.35 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD13 | 10 | 0.35 |
| (2,1262) | 2:B:155:ILE:HG12 | 1:A:7:LEU:HD22 | 10 | 0.35 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD12 | 10 | 0.35 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD11 | 10 | 0.35 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD13 | 10 | 0.35 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD22 | 10 | 0.35 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD21 | 10 | 0.35 |
| (2,1262) | 2:B:155:ILE:HG13 | 1:A:7:LEU:HD23 | 10 | 0.35 |
| (2,855) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 1 | 0.34 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 1 | 0.34 |
| (2,855) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 1 | 0.34 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 1 | 0.34 |
| (2,855) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 1 | 0.34 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 2 | 0.34 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 2 | 0.34 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 2 | 0.34 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 2 | 0.34 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 4 | 0.34 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 10 | 0.34 |
| (2,3430) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 6 | 0.34 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 6 | 0.34 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 6 | 0.34 |
| (2,3203) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 8 | 0.34 |
| (2,3203) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 8 | 0.34 |
| (2,3203) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 8 | 0.34 |
| (2,3203) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 8 | 0.34 |
| (2,3106) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 9 | 0.34 |
| (2,3106) | 2:B:146:LEU:HD13 | 2:B:142:VAL:HA | 9 | 0.34 |
| (2,3106) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 9 | 0.34 |
| (2,3106) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 9 | 0.34 |
| (2,3017) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 6 | 0.34 |
| (2,3017) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 6 | 0.34 |
| (2,3017) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 6 | 0.34 |
| (2,3017) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 6 | 0.34 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 9 | 0.34 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 9 | 0.34 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 9 | 0.34 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 9 | 0.34 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 2 | 0.34 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 2 | 0.34 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 2 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 2 | 0.34 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 2 | 0.34 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 2 | 0.34 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 2 | 0.34 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 2 | 0.34 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 5 | 0.34 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 5 | 0.34 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 5 | 0.34 |
| (2,1654) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 5 | 0.34 |
| (2,1654) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 5 | 0.34 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 5 | 0.34 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 5 | 0.34 |
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 5 | 0.34 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 5 | 0.34 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 5 | 0.34 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 5 | 0.34 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 8 | 0.34 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 8 | 0.34 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 8 | 0.34 |
| (2,1087) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 8 | 0.34 |
| (2,558) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 4 | 0.33 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 4 | 0.33 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 4 | 0.33 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 10 | 0.33 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 1 | 0.33 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 2 | 0.33 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 4 | 0.33 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 7 | 0.33 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 8 | 0.33 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 10 | 0.33 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 8 | 0.33 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 8 | 0.33 |
| (2,3858) | 2:B:125:LYS:H | 2:B:125:LYS:HB2 | 10 | 0.33 |
| (2,3394) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HG | 4 | 0.33 |
| (2,3394) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HG | 4 | 0.33 |
| (2,3394) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HG | 4 | 0.33 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 3 | 0.33 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 3 | 0.33 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 3 | 0.33 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 8 | 0.33 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 8 | 0.33 |
| (2,2979) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 8 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2979) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 8 | 0.33 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 4 | 0.33 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 4 | 0.33 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 2 | 0.33 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 2 | 0.33 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 2 | 0.33 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 1 | 0.33 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 1 | 0.33 |
| (2,2257) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD21 | 5 | 0.33 |
| (2,2257) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD22 | 5 | 0.33 |
| (2,2257) | 1:A:25:GLU:HG3 | 1:A:29:ASN:HD22 | 5 | 0.33 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 7 | 0.33 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 7 | 0.33 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.33 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.33 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.33 |
| (2,1648) | 2:B:109:LEU:HA | 2:B:109:LEU:HD12 | 4 | 0.33 |
| (2,1648) | 2:B:109:LEU:HA | 2:B:109:LEU:HD13 | 4 | 0.33 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG12 | 8 | 0.33 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG11 | 8 | 0.33 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG13 | 8 | 0.33 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG22 | 8 | 0.33 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG23 | 8 | 0.33 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB2 | 2 | 0.32 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB1 | 2 | 0.32 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB3 | 2 | 0.32 |
| (2,493) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB1 | 2 | 0.32 |
| (2,493) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB3 | 2 | 0.32 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 2 | 0.32 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 4 | 0.32 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 7 | 0.32 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 8 | 0.32 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 3 | 0.32 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 6 | 0.32 |
| (2,4203) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 8 | 0.32 |
| (2,4159) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 7 | 0.32 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 9 | 0.32 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 1 | 0.32 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 1 | 0.32 |
| (2,3502) | 2:B:159:ILE:HD12 | 1:A:60:ILE:HG13 | 10 | 0.32 |
| (2,3502) | 2:B:159:ILE:HD11 | 1:A:60:ILE:HG13 | 10 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 2 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 2 | 0.32 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 2 | 0.32 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 1 | 0.32 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 1 | 0.32 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 1 | 0.32 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 6 | 0.32 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 6 | 0.32 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 6 | 0.32 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 2 | 0.32 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 2 | 0.32 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 10 | 0.32 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 10 | 0.32 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 10 | 0.32 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB3 | 10 | 0.32 |
| (2,1994) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HB3 | 10 | 0.32 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB2 | 10 | 0.32 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 2 | 0.32 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 2 | 0.32 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD12 | 9 | 0.32 |
| (2,1159) | 2:B:152:GLU:HA | 2:B:155:ILE:HD11 | 9 | 0.32 |
| (2,790) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 10 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 10 | 0.31 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 10 | 0.31 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 7 | 0.31 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 7 | 0.31 |
| (2,784) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 7 | 0.31 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 9 | 0.31 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 1 | 0.31 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 5 | 0.31 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 6 | 0.31 |
| (2,341) | 1:A:1:MET:HG2 | 1:A:7:LEU:HD12 | 1 | 0.31 |
| (2,341) | 1:A:1:MET:HG2 | 1:A:7:LEU:HD11 | 1 | 0.31 |
| (2,341) | 1:A:1:MET:HG2 | 1:A:7:LEU:HD13 | 1 | 0.31 |
| (2,341) | 1:A:1:MET:HG2 | 1:A:7:LEU:HD22 | 1 | 0.31 |
| (2,341) | 1:A:1:MET:HG2 | 1:A:7:LEU:HD21 | 1 | 0.31 |
| (2,341) | 1:A:1:MET:HG2 | 1:A:7:LEU:HD23 | 1 | 0.31 |
| (2,341) | 1:A:1:MET:HG3 | 1:A:7:LEU:HD21 | 1 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 5 | 0.31 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 5 | 0.31 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 10 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 10 | 0.31 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 10 | 0.31 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 7 | 0.31 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 7 | 0.31 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 7 | 0.31 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 9 | 0.31 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 9 | 0.31 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD12 | 10 | 0.31 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD13 | 10 | 0.31 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD22 | 10 | 0.31 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 10 | 0.31 |
| (2,3111) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB2 | 10 | 0.31 |
| (2,3111) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB3 | 10 | 0.31 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 10 | 0.31 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 7 | 0.31 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 7 | 0.31 |
| (2,2627) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 7 | 0.31 |
| (2,2627) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 7 | 0.31 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 10 | 0.31 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 10 | 0.31 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 10 | 0.31 |
| (2,2593) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 10 | 0.31 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 6 | 0.31 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 6 | 0.31 |
| (2,2571) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 6 | 0.31 |
| (2,2571) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 6 | 0.31 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 6 | 0.31 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 6 | 0.31 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 10 | 0.31 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 10 | 0.31 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.31 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.31 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD12 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD11 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD13 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD12 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD11 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD13 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD12 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD11 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD13 | 2 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD12 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD11 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD13 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD12 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD11 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD13 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD11 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD13 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD11 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD13 | 2 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD12 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD11 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD12 | 2:B:143:ILE:HD13 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD12 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD11 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD11 | 2:B:143:ILE:HD13 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD12 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD11 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD13 | 2:B:143:ILE:HD13 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD12 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD11 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:123:ILE:HD13 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD12 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD11 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD22 | 2:B:143:ILE:HD13 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD11 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:123:ILE:HD13 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD11 | 8 | 0.31 |
| (2,1843) | 2:B:139:LEU:HD23 | 2:B:143:ILE:HD13 | 8 | 0.31 |
| (2,586) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 3 | 0.3 |
| (2,586) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 3 | 0.3 |
| (2,586) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 3 | 0.3 |
| (2,586) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 3 | 0.3 |
| (2,586) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 3 | 0.3 |
| (2,558) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 5 | 0.3 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 5 | 0.3 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 5 | 0.3 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 6 | 0.3 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 6 | 0.3 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 6 | 0.3 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 6 | 0.3 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 6 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 6 | 0.3 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 2 | 0.3 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 4 | 0.3 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 7 | 0.3 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 8 | 0.3 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 10 | 0.3 |
| (2,4181) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 5 | 0.3 |
| (2,4181) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 6 | 0.3 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 1 | 0.3 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 3 | 0.3 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 5 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 2 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 2 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 2 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 4 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 4 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 4 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 9 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 9 | 0.3 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 9 | 0.3 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 7 | 0.3 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 7 | 0.3 |
| (2,2636) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 7 | 0.3 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 1 | 0.3 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 1 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 3 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 4 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 4 | 0.3 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 4 | 0.3 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE2 | 6 | 0.3 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE3 | 6 | 0.3 |
| (2,1716) | 2:B:121:LYS:HG3 | 2:B:121:LYS:HE3 | 6 | 0.3 |
| (2,1700) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 3 | 0.3 |
| (2,1700) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 3 | 0.3 |
| (2,1700) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 3 | 0.3 |
| (2,1700) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 3 | 0.3 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 2 | 0.3 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 2 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 8 | 0.3 |
| (2,1625) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 8 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG12 | 6 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG11 | 6 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG13 | 6 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG22 | 6 | 0.3 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG23 | 6 | 0.3 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 9 | 0.3 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 6 | 0.29 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 6 | 0.29 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 6 | 0.29 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB2 | 5 | 0.29 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB1 | 5 | 0.29 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB3 | 5 | 0.29 |
| (2,493) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB1 | 5 | 0.29 |
| (2,493) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB3 | 5 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 1 | 0.29 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 3 | 0.29 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 3 | 0.29 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 4 | 0.29 |
| (2,4122) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 5 | 0.29 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 3 | 0.29 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 3 | 0.29 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 9 | 0.29 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 9 | 0.29 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 3 | 0.29 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 3 | 0.29 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 3 | 0.29 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 6 | 0.29 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 6 | 0.29 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 6 | 0.29 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG2 | 4 | 0.29 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG3 | 4 | 0.29 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 4 | 0.29 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 4 | 0.29 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 4 | 0.29 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 4 | 0.29 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 4 | 0.29 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 9 | 0.29 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 9 | 0.29 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 9 | 0.29 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 9 | 0.29 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 9 | 0.29 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 5 | 0.29 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 5 | 0.29 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 5 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 3 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 3 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 3 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 3 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 3 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 6 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 6 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 6 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 6 | 0.29 |
| (2,3021) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 6 | 0.29 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 9 | 0.29 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 9 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2979) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 9 | 0.29 |
| (2,2979) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 9 | 0.29 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 4 | 0.29 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 4 | 0.29 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 4 | 0.29 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 4 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 8 | 0.29 |
| (2,2645) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 8 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 7 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 7 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 7 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 7 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 7 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 7 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 9 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 9 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 9 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 9 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 9 | 0.29 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 9 | 0.29 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 7 | 0.29 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 7 | 0.29 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 7 | 0.29 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 7 | 0.29 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 7 | 0.29 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 7 | 0.29 |
| (2,2256) | 1:A:25:GLU:HG3 | 1:A:29:ASN:HD22 | 9 | 0.29 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD21 | 9 | 0.29 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD22 | 9 | 0.29 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 1 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 1 | 0.29 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 1 | 0.29 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 4 | 0.29 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 4 | 0.29 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 4 | 0.29 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 8 | 0.29 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 8 | 0.29 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 8 | 0.29 |
| (2,1944) | 2:B:154:VAL:HG12 | 2:B:154:VAL:HA | 9 | 0.29 |
| (2,1944) | 2:B:154:VAL:HG13 | 2:B:154:VAL:HA | 9 | 0.29 |
| (2,1944) | 2:B:154:VAL:HG22 | 2:B:154:VAL:HA | 9 | 0.29 |
| (2,1944) | 2:B:154:VAL:HG21 | 2:B:154:VAL:HA | 9 | 0.29 |
| (2,1936) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 8 | 0.29 |
| (2,1936) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 8 | 0.29 |
| (2,1936) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 8 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 2 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 9 | 0.29 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.29 |
| (2,1899) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.29 |
| (2,1721) | 2:B:122:ASP:HA | 2:B:125:LYS:HG2 | 5 | 0.29 |
| (2,1721) | 2:B:122:ASP:HA | 2:B:125:LYS:HG3 | 5 | 0.29 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 4 | 0.29 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 4 | 0.29 |
| (2,1102) | 2:B:143:ILE:HD12 | 2:B:107:TYR:HD2 | 1 | 0.29 |
| (2,1102) | 2:B:143:ILE:HD11 | 2:B:107:TYR:HD2 | 1 | 0.29 |
| (2,1102) | 2:B:143:ILE:HD13 | 2:B:107:TYR:HD2 | 1 | 0.29 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 10 | 0.29 |
| (2,4555) | 2:B:159:ILE:HA | 2:B:159:ILE:HG12 | 5 | 0.28 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 6 | 0.28 |
| (2,4528) | 2:B:151:ILE:HA | 2:B:151:ILE:HG12 | 9 | 0.28 |
| (2,4186) | 2:B:127:LEU:HG | 2:B:124:LYS:HD2 | 5 | 0.28 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 8 | 0.28 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 7 | 0.28 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 7 | 0.28 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 10 | 0.28 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 10 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 4 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 4 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 4 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 8 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 8 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 8 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 9 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 9 | 0.28 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 9 | 0.28 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 3 | 0.28 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 3 | 0.28 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 3 | 0.28 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 3 | 0.28 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 3 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 3 | 0.28 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 3 | 0.28 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 3 | 0.28 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 3 | 0.28 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 3 | 0.28 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 2 | 0.28 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 2 | 0.28 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 7 | 0.28 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 7 | 0.28 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG22 | 4 | 0.28 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG21 | 4 | 0.28 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG21 | 4 | 0.28 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG23 | 4 | 0.28 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG22 | 10 | 0.28 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG21 | 10 | 0.28 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG21 | 10 | 0.28 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG23 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.28 |
| (2,3095) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.28 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.28 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.28 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 5 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 5 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 5 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 5 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 5 | 0.28 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 5 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,217) | 2:B:117:SER:H | 2:B:115:ASN:HD21 | 2 | 0.28 |
| (2,217) | 2:B:117:SER:H | 2:B:115:ASN:HD22 | 2 | 0.28 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 4 | 0.28 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 4 | 0.28 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 5 | 0.28 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 5 | 0.28 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 9 | 0.28 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 9 | 0.28 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 2 | 0.28 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 2 | 0.28 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 2 | 0.28 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 7 | 0.28 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 7 | 0.28 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 7 | 0.28 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB3 | 4 | 0.28 |
| (2,1994) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HB3 | 4 | 0.28 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB2 | 4 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 5 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 7 | 0.28 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 7 | 0.28 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 9 | 0.28 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 9 | 0.28 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 9 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,186) | 2:B:111:ALA:H | 2:B:109:LEU:HD12 | 4 | 0.28 |
| (2,186) | 2:B:111:ALA:H | 2:B:109:LEU:HD11 | 4 | 0.28 |
| (2,186) | 2:B:111:ALA:H | 2:B:109:LEU:HD13 | 4 | 0.28 |
| (2,186) | 2:B:111:ALA:H | 1:A:37:VAL:HG12 | 4 | 0.28 |
| (2,186) | 2:B:111:ALA:H | 1:A:37:VAL:HG11 | 4 | 0.28 |
| (2,186) | 2:B:111:ALA:H | 1:A:37:VAL:HG13 | 4 | 0.28 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 4 | 0.28 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 4 | 0.28 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 4 | 0.28 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 7 | 0.28 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 7 | 0.28 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 7 | 0.28 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 6 | 0.28 |
| (2,1715) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 6 | 0.28 |
| (2,1715) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 6 | 0.28 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 1 | 0.28 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 1 | 0.28 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 3 | 0.28 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 3 | 0.28 |
| (2,1658) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HG13 | 1 | 0.28 |
| (2,1658) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HG13 | 1 | 0.28 |
| (2,1658) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HG13 | 1 | 0.28 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.28 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.28 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.28 |
| (2,1059) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 6 | 0.28 |
| (2,1059) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 6 | 0.28 |
| (2,1059) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 6 | 0.28 |
| (2,1059) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 6 | 0.28 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 7 | 0.27 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 7 | 0.27 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 7 | 0.27 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 1 | 0.27 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 1 | 0.27 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 1 | 0.27 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 1 | 0.27 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 1 | 0.27 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 1 | 0.27 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 1 | 0.27 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 5 | 0.27 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 5 | 0.27 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 5 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB2 | 9 | 0.27 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB1 | 9 | 0.27 |
| (2,493) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB3 | 9 | 0.27 |
| (2,493) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB1 | 9 | 0.27 |
| (2,493) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB3 | 9 | 0.27 |
| (2,4566) | 2:B:165:VAL:H | 2:B:165:VAL:HB | 9 | 0.27 |
| (2,4391) | 1:A:61:CYS:HA | 1:A:62:ASN:HA | 3 | 0.27 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 2 | 0.27 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 10 | 0.27 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 1 | 0.27 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 1 | 0.27 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 6 | 0.27 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 6 | 0.27 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 10 | 0.27 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 10 | 0.27 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 4 | 0.27 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 7 | 0.27 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 7 | 0.27 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 7 | 0.27 |
| (2,3446) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,3446) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,3446) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,3446) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,3446) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,3430) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 7 | 0.27 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 7 | 0.27 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 7 | 0.27 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 9 | 0.27 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 9 | 0.27 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 2 | 0.27 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 2 | 0.27 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 2 | 0.27 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 2 | 0.27 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 2 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 7 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 7 | 0.27 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 7 | 0.27 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 3 | 0.27 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 3 | 0.27 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 3 | 0.27 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 6 | 0.27 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 6 | 0.27 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 6 | 0.27 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 10 | 0.27 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 10 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 2 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 2 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 2 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 2 | 0.27 |
| (2,3021) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 2 | 0.27 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 7 | 0.27 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 7 | 0.27 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 7 | 0.27 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 10 | 0.27 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 10 | 0.27 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 10 | 0.27 |
| (2,2738) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,2738) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,2738) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,2738) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,2738) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 10 | 0.27 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 8 | 0.27 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 8 | 0.27 |
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 8 | 0.27 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 10 | 0.27 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 10 | 0.27 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 10 | 0.27 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 10 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 10 | 0.27 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 10 | 0.27 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE2 | 7 | 0.27 |
| (2,2450) | 1:A:46:LEU:HB3 | 1:A:49:LYS:HE3 | 7 | 0.27 |
| (2,2450) | 1:A:46:LEU:HB2 | 1:A:49:LYS:HE3 | 7 | 0.27 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 4 | 0.27 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 4 | 0.27 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 6 | 0.27 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 6 | 0.27 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 9 | 0.27 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 9 | 0.27 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 9 | 0.27 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 9 | 0.27 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 8 | 0.27 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 8 | 0.27 |
| (2,2328) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 8 | 0.27 |
| (2,217) | 2:B:117:SER:H | 2:B:115:ASN:HD21 | 10 | 0.27 |
| (2,217) | 2:B:117:SER:H | 2:B:115:ASN:HD22 | 10 | 0.27 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 10 | 0.27 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 10 | 0.27 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 10 | 0.27 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 10 | 0.27 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 10 | 0.27 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 3 | 0.27 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 3 | 0.27 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 2 | 0.27 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 2 | 0.27 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.27 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG21 | 2:B:149:LYS:HD3 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG13 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG23 | 2:B:149:LYS:HD3 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG12 | 2:B:155:ILE:HG12 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG11 | 2:B:155:ILE:HG12 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG13 | 2:B:155:ILE:HG12 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD2 | 6 | 0.27 |
| (2,1948) | 2:B:154:VAL:HG22 | 2:B:149:LYS:HD3 | 6 | 0.27 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 2 | 0.27 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 2 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 2 | 0.27 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 2 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 2 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 2 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 2 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 3 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 3 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 3 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 8 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 8 | 0.27 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 8 | 0.27 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 9 | 0.27 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 9 | 0.27 |
| (2,1598) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 3 | 0.27 |
| (2,1598) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 3 | 0.27 |
| (2,1598) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 3 | 0.27 |
| (2,1598) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 3 | 0.27 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 6 | 0.27 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 6 | 0.27 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 6 | 0.27 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 7 | 0.27 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 7 | 0.27 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.27 |
| (2,1127) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.27 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 6 | 0.26 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 6 | 0.26 |
| (2,920) | 2:B:122:ASP:HA | 2:B:125:LYS:HG2 | 5 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,920) | 2:B:122:ASP:HA | 2:B:125:LYS:HG3 | 5 | 0.26 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 6 | 0.26 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 6 | 0.26 |
| (2,847) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 6 | 0.26 |
| (2,847) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 6 | 0.26 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 1 | 0.26 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 1 | 0.26 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 1 | 0.26 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 2 | 0.26 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 2 | 0.26 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 2 | 0.26 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 2 | 0.26 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 2 | 0.26 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 2 | 0.26 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 7 | 0.26 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 7 | 0.26 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 7 | 0.26 |
| (2,558) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 9 | 0.26 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 9 | 0.26 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 9 | 0.26 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 1 | 0.26 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 1 | 0.26 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 1 | 0.26 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 1 | 0.26 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 1 | 0.26 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 3 | 0.26 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 3 | 0.26 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 7 | 0.26 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 1 | 0.26 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 4 | 0.26 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 6 | 0.26 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 8 | 0.26 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 6 | 0.26 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 8 | 0.26 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 5 | 0.26 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 5 | 0.26 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 8 | 0.26 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 8 | 0.26 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 4 | 0.26 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 8 | 0.26 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 3 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 5 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,3446) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,3446) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,3385) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 3 | 0.26 |
| (2,3385) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 3 | 0.26 |
| (2,3385) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 3 | 0.26 |
| (2,3385) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 3 | 0.26 |
| (2,3385) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 3 | 0.26 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 5 | 0.26 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 5 | 0.26 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 2 | 0.26 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 2 | 0.26 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 10 | 0.26 |
| (2,3156) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 10 | 0.26 |
| (2,3156) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 10 | 0.26 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 1 | 0.26 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 1 | 0.26 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 1 | 0.26 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 1 | 0.26 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 5 | 0.26 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 5 | 0.26 |
| (2,2979) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 5 | 0.26 |
| (2,2979) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 5 | 0.26 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 6 | 0.26 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 6 | 0.26 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 2 | 0.26 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 2 | 0.26 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 2 | 0.26 |
| (2,282) | 2:B:140:ASN:H | 2:B:141:LYS:HB2 | 3 | 0.26 |
| (2,282) | 2:B:140:ASN:H | 2:B:141:LYS:HB3 | 3 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,2738) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 5 | 0.26 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 5 | 0.26 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 5 | 0.26 |
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 5 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 1 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 1 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 2 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 2 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 5 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 5 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 7 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 7 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 8 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 8 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 10 | 0.26 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 10 | 0.26 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 4 | 0.26 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 4 | 0.26 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 4 | 0.26 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 4 | 0.26 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 2 | 0.26 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 2 | 0.26 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 2 | 0.26 |
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 2 | 0.26 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 9 | 0.26 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 9 | 0.26 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 9 | 0.26 |
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 9 | 0.26 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 3 | 0.26 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 3 | 0.26 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 3 | 0.26 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG22 | 3 | 0.26 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG21 | 3 | 0.26 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG23 | 3 | 0.26 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG12 | 3 | 0.26 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG11 | 3 | 0.26 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG22 | 3 | 0.26 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG21 | 3 | 0.26 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG23 | 3 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 4 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 4 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 6 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 6 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 7 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 7 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 8 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 8 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 9 | 0.26 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 9 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG2 | 4 | 0.26 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG3 | 4 | 0.26 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 9 | 0.26 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 9 | 0.26 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 9 | 0.26 |
| (2,1765) | 2:B:126:ILE:HD12 | 2:B:125:LYS:HD2 | 8 | 0.26 |
| (2,1765) | 2:B:126:ILE:HD12 | 2:B:125:LYS:HD3 | 8 | 0.26 |
| (2,1765) | 2:B:126:ILE:HD11 | 2:B:125:LYS:HD2 | 8 | 0.26 |
| (2,1765) | 2:B:126:ILE:HD11 | 2:B:125:LYS:HD3 | 8 | 0.26 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 9 | 0.26 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 9 | 0.26 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 9 | 0.26 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG12 | 4 | 0.26 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG11 | 4 | 0.26 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG13 | 4 | 0.26 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG22 | 4 | 0.26 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG23 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 1 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 2 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 3 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 3 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 4 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 5 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 6 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 7 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 7 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 8 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 9 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD11 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD12 | 1:A:7:LEU:HD13 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD11 | 1:A:7:LEU:HD13 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD21 | 10 | 0.26 |
| (2,1298) | 1:A:7:LEU:HD22 | 1:A:7:LEU:HD23 | 10 | 0.26 |
| (2,1251) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD3 | 7 | 0.26 |
| (2,1251) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD2 | 7 | 0.26 |
| (2,1251) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD2 | 7 | 0.26 |
| (2,1251) | 2:B:165:VAL:HG13 | 2:B:166:PRO:HD2 | 7 | 0.26 |
| (2,1251) | 2:B:165:VAL:HG12 | 2:B:166:PRO:HD3 | 7 | 0.26 |
| (2,1251) | 2:B:165:VAL:HG11 | 2:B:166:PRO:HD3 | 7 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 6 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 6 | 0.26 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 6 | 0.26 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD12 | 6 | 0.26 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD13 | 6 | 0.26 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD22 | 6 | 0.26 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 6 | 0.26 |
| (2,1136) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB2 | 6 | 0.26 |
| (2,1136) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB3 | 6 | 0.26 |
| (2,1136) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 6 | 0.26 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD11 | 6 | 0.26 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD13 | 6 | 0.26 |
| (2,1132) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 6 | 0.26 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD21 | 6 | 0.26 |
| (2,1132) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 6 | 0.26 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD12 | 6 | 0.26 |
| (2,1132) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 6 | 0.26 |
| (2,1102) | 2:B:143:ILE:HD12 | 2:B:107:TYR:HD2 | 10 | 0.26 |
| (2,1102) | 2:B:143:ILE:HD11 | 2:B:107:TYR:HD2 | 10 | 0.26 |
| (2,1102) | 2:B:143:ILE:HD13 | 2:B:107:TYR:HD2 | 10 | 0.26 |
| (2,1060) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HD2 | 6 | 0.26 |
| (2,1060) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HD2 | 6 | 0.26 |
| (2,1060) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HD2 | 6 | 0.26 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 8 | 0.26 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 8 | 0.26 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 8 | 0.26 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 2 | 0.26 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 4 | 0.25 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 8 | 0.25 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 8 | 0.25 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 7 | 0.25 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 7 | 0.25 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 7 | 0.25 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 7 | 0.25 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 3 | 0.25 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 3 | 0.25 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 3 | 0.25 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 9 | 0.25 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 9 | 0.25 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 9 | 0.25 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 4 | 0.25 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 4 | 0.25 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 4 | 0.25 |
| (2,619) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 6 | 0.25 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 6 | 0.25 |
| (2,619) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 6 | 0.25 |
| (2,558) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 10 | 0.25 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 10 | 0.25 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 10 | 0.25 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD11 | 8 | 0.25 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD13 | 8 | 0.25 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD11 | 8 | 0.25 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD13 | 8 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 2 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 2 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 2 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 5 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 5 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 5 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 6 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 6 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 6 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 7 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 7 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 7 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 10 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 10 | 0.25 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 10 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 4 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 4 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 4 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 4 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 8 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 8 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 8 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 8 | 0.25 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 8 | 0.25 |
| (2,4391) | 1:A:61:CYS:HA | 1:A:62:ASN:HA | 1 | 0.25 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 1 | 0.25 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 2 | 0.25 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 3 | 0.25 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 4 | 0.25 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 5 | 0.25 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 8 | 0.25 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 9 | 0.25 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 10 | 0.25 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 7 | 0.25 |
| (2,4113) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 7 | 0.25 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 6 | 0.25 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 6 | 0.25 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 7 | 0.25 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 1 | 0.25 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 2 | 0.25 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 5 | 0.25 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 7 | 0.25 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 10 | 0.25 |
| (2,3999) | 2:B:160:GLY:H | 2:B:162:LEU:H | 1 | 0.25 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 1 | 0.25 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 1 | 0.25 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 9 | 0.25 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 9 | 0.25 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 9 | 0.25 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 3 | 0.25 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 7 | 0.25 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 8 | 0.25 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 6 | 0.25 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 2 | 0.25 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 5 | 0.25 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 6 | 0.25 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 10 | 0.25 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 5 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 5 | 0.25 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 5 | 0.25 |
| (2,3492) | 2:B:152:GLU:HG2 | 1:A:7:LEU:HB3 | 3 | 0.25 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB2 | 3 | 0.25 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB3 | 3 | 0.25 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 9 | 0.25 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 9 | 0.25 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 9 | 0.25 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 9 | 0.25 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 9 | 0.25 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 9 | 0.25 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 9 | 0.25 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 9 | 0.25 |
| (2,3416) | 2:B:101:MET:HE2 | 1:A:17:HIS:HD2 | 1 | 0.25 |
| (2,3416) | 2:B:101:MET:HE1 | 1:A:17:HIS:HD2 | 1 | 0.25 |
| (2,3416) | 2:B:101:MET:HE3 | 1:A:17:HIS:HD2 | 1 | 0.25 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 9 | 0.25 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 9 | 0.25 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 1 | 0.25 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 1 | 0.25 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 8 | 0.25 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 8 | 0.25 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 5 | 0.25 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 5 | 0.25 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 5 | 0.25 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 7 | 0.25 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 7 | 0.25 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 7 | 0.25 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 4 | 0.25 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 4 | 0.25 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 4 | 0.25 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 4 | 0.25 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 4 | 0.25 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 4 | 0.25 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 8 | 0.25 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 8 | 0.25 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 4 | 0.25 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 4 | 0.25 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 9 | 0.25 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 9 | 0.25 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 6 | 0.25 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 6 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 6 | 0.25 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 3 | 0.25 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 3 | 0.25 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB2 | 9 | 0.25 |
| (2,2438) | 1:A:43:TRP:HE1 | 1:A:43:TRP:HB3 | 9 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 1 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 1 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 1 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 1 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 1 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 1 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 5 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 5 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 5 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 5 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 5 | 0.25 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 5 | 0.25 |
| (2,2373) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 1 | 0.25 |
| (2,2373) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 1 | 0.25 |
| (2,2373) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 1 | 0.25 |
| (2,2373) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 1 | 0.25 |
| (2,2373) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 1 | 0.25 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 2 | 0.25 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 2 | 0.25 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 2 | 0.25 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 2 | 0.25 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG22 | 2 | 0.25 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG21 | 2 | 0.25 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG23 | 2 | 0.25 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD21 | 2 | 0.25 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD23 | 2 | 0.25 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG22 | 2 | 0.25 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG21 | 2 | 0.25 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG23 | 2 | 0.25 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 4 | 0.25 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 4 | 0.25 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 4 | 0.25 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 6 | 0.25 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 6 | 0.25 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 6 | 0.25 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 5 | 0.25 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 5 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 5 | 0.25 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 9 | 0.25 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 9 | 0.25 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 5 | 0.25 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 5 | 0.25 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 5 | 0.25 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 5 | 0.25 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 1 | 0.25 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 1 | 0.25 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 1 | 0.25 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 1 | 0.25 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 2 | 0.25 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 2 | 0.25 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 2 | 0.25 |
| (2,1809) | 2:B:132:ILE:HG22 | 1:A:18:ASP:HB2 | 6 | 0.25 |
| (2,1809) | 2:B:132:ILE:HG23 | 1:A:18:ASP:HB2 | 6 | 0.25 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 10 | 0.25 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 10 | 0.25 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 10 | 0.25 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 4 | 0.25 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 4 | 0.25 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 4 | 0.25 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 4 | 0.25 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 4 | 0.25 |
| (2,1598) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD11 | 5 | 0.25 |
| (2,1598) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD11 | 5 | 0.25 |
| (2,1598) | 1:A:57:GLY:HA2 | 1:A:60:ILE:HD13 | 5 | 0.25 |
| (2,1598) | 1:A:57:GLY:HA3 | 1:A:60:ILE:HD13 | 5 | 0.25 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 6 | 0.25 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 6 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 1 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 1 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 1 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 2 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 2 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 2 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 3 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 3 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 3 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 4 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 4 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 5 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 5 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 5 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 8 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 8 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 8 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 9 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 9 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 9 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG23 | 2:B:151:ILE:HG13 | 10 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG12 | 10 | 0.25 |
| (2,1157) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HG13 | 10 | 0.25 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD11 | 1 | 0.25 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD13 | 1 | 0.25 |
| (2,1132) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 1 | 0.25 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD21 | 1 | 0.25 |
| (2,1132) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 1 | 0.25 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD12 | 1 | 0.25 |
| (2,1132) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 1 | 0.25 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD11 | 4 | 0.25 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD13 | 4 | 0.25 |
| (2,1132) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 4 | 0.25 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD21 | 4 | 0.25 |
| (2,1132) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 4 | 0.25 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD12 | 4 | 0.25 |
| (2,1132) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 4 | 0.25 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 5 | 0.25 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 6 | 0.25 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 7 | 0.25 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 9 | 0.24 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 9 | 0.24 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 5 | 0.24 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 5 | 0.24 |
| (2,847) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 5 | 0.24 |
| (2,847) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 5 | 0.24 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 8 | 0.24 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 8 | 0.24 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 8 | 0.24 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 9 | 0.24 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 9 | 0.24 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 9 | 0.24 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 6 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 6 | 0.24 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 6 | 0.24 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 6 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 1 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 1 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 1 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 3 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 3 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 3 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 4 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 4 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 4 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 8 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 8 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 8 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG21 | 9 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG22 | 9 | 0.24 |
| (2,471) | 1:A:22:THR:HB | 1:A:22:THR:HG23 | 9 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 9 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 9 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 9 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 9 | 0.24 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 9 | 0.24 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 5 | 0.24 |
| (2,4556) | 2:B:161:LYS:HA | 2:B:161:LYS:H | 4 | 0.24 |
| (2,4556) | 2:B:161:LYS:HA | 2:B:161:LYS:H | 9 | 0.24 |
| (2,4556) | 2:B:161:LYS:HA | 2:B:161:LYS:H | 10 | 0.24 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 1 | 0.24 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 4 | 0.24 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 7 | 0.24 |
| (2,4373) | 1:A:59:LEU:HB3 | 1:A:59:LEU:H | 6 | 0.24 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 3 | 0.24 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 5 | 0.24 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 9 | 0.24 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 4 | 0.24 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 4 | 0.24 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 3 | 0.24 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 4 | 0.24 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 6 | 0.24 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 8 | 0.24 |
| (2,4015) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 9 | 0.24 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 6 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 9 | 0.24 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 10 | 0.24 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 1 | 0.24 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 1 | 0.24 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 1 | 0.24 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 10 | 0.24 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 10 | 0.24 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 10 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 3 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 6 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 8 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 8 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 8 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 8 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 8 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 8 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 8 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 8 | 0.24 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 8 | 0.24 |
| (2,334) | 2:B:167:ALA:H | 2:B:167:ALA:HB2 | 8 | 0.24 |
| (2,334) | 2:B:167:ALA:H | 2:B:167:ALA:HB1 | 8 | 0.24 |
| (2,334) | 2:B:167:ALA:H | 2:B:167:ALA:HB3 | 8 | 0.24 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 5 | 0.24 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 5 | 0.24 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 3 | 0.24 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 3 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG2 | 10 | 0.24 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG3 | 10 | 0.24 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 1 | 0.24 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 1 | 0.24 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD12 | 4 | 0.24 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD11 | 4 | 0.24 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD13 | 4 | 0.24 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD12 | 10 | 0.24 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD11 | 10 | 0.24 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD13 | 10 | 0.24 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.24 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.24 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.24 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 9 | 0.24 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 9 | 0.24 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 4 | 0.24 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 4 | 0.24 |
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 4 | 0.24 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 2 | 0.24 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 2 | 0.24 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 2 | 0.24 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 2 | 0.24 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 3 | 0.24 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 3 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 3 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 3 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 3 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 3 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 3 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 3 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 9 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 9 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 9 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 9 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 9 | 0.24 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 9 | 0.24 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 9 | 0.24 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 9 | 0.24 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 9 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 4 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 4 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 4 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 4 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 5 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 5 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 5 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 5 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 7 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 7 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 7 | 0.24 |
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 7 | 0.24 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 9 | 0.24 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 9 | 0.24 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 9 | 0.24 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 8 | 0.24 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 8 | 0.24 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 1 | 0.24 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 1 | 0.24 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 3 | 0.24 |
| (2,1980) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 3 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG12 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG13 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD2 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD3 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG12 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG13 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HD3 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:151:ILE:HG12 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HD3 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG12 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG13 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:155:ILE:HG12 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG12 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG13 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HD3 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG12 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG13 | 8 | 0.24 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HD3 | 8 | 0.24 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 4 | 0.24 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 4 | 0.24 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 4 | 0.24 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 4 | 0.24 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE2 | 1 | 0.24 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE3 | 1 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1716) | 2:B:121:LYS:HG3 | 2:B:121:LYS:HE3 | 1 | 0.24 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE2 | 3 | 0.24 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE3 | 3 | 0.24 |
| (2,1716) | 2:B:121:LYS:HG3 | 2:B:121:LYS:HE3 | 3 | 0.24 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 1 | 0.24 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 1 | 0.24 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 3 | 0.24 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 3 | 0.24 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 5 | 0.24 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 5 | 0.24 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 6 | 0.24 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 6 | 0.24 |
| (2,1700) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 2 | 0.24 |
| (2,1700) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 2 | 0.24 |
| (2,1700) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 2 | 0.24 |
| (2,1700) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 2 | 0.24 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG12 | 1 | 0.24 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG11 | 1 | 0.24 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG13 | 1 | 0.24 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG22 | 1 | 0.24 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG23 | 1 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 10 | 0.24 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 10 | 0.24 |
| (2,1102) | 2:B:143:ILE:HD12 | 2:B:107:TYR:HD2 | 3 | 0.24 |
| (2,1102) | 2:B:143:ILE:HD11 | 2:B:107:TYR:HD2 | 3 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1102) | 2:B:143:ILE:HD13 | 2:B:107:TYR:HD2 | 3 | 0.24 |
| (2,1102) | 2:B:143:ILE:HD12 | 2:B:107:TYR:HD2 | 4 | 0.24 |
| (2,1102) | 2:B:143:ILE:HD11 | 2:B:107:TYR:HD2 | 4 | 0.24 |
| (2,1102) | 2:B:143:ILE:HD13 | 2:B:107:TYR:HD2 | 4 | 0.24 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 4 | 0.24 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 4 | 0.24 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 4 | 0.24 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 3 | 0.24 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 8 | 0.24 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 3 | 0.24 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 7 | 0.24 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 3 | 0.23 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 3 | 0.23 |
| (2,846) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 8 | 0.23 |
| (2,846) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 8 | 0.23 |
| (2,846) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 8 | 0.23 |
| (2,846) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 8 | 0.23 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 4 | 0.23 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 4 | 0.23 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 4 | 0.23 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 7 | 0.23 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 7 | 0.23 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG22 | 4 | 0.23 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG21 | 4 | 0.23 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG23 | 4 | 0.23 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HD12 | 4 | 0.23 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG22 | 4 | 0.23 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG21 | 4 | 0.23 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG23 | 4 | 0.23 |
| (2,567) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG22 | 4 | 0.23 |
| (2,567) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG21 | 4 | 0.23 |
| (2,522) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 3 | 0.23 |
| (2,522) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 3 | 0.23 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG2 | 10 | 0.23 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG3 | 10 | 0.23 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 7 | 0.23 |
| (2,4556) | 2:B:161:LYS:HA | 2:B:161:LYS:H | 7 | 0.23 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 6 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 1 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 2 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 3 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 4 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 5 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 7 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 8 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 9 | 0.23 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 10 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 1 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 2 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 3 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 4 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 5 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 6 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 7 | 0.23 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 10 | 0.23 |
| (2,4119) | 2:B:155:ILE:HB | 2:B:152:GLU:HA | 3 | 0.23 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 2 | 0.23 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 2 | 0.23 |
| (2,4002) | 2:B:165:VAL:H | 2:B:165:VAL:HB | 9 | 0.23 |
| (2,391) | 1:A:10:ILE:HG22 | 2:B:159:ILE:HG12 | 2 | 0.23 |
| (2,391) | 1:A:10:ILE:HG23 | 2:B:159:ILE:HG12 | 2 | 0.23 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 8 | 0.23 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 8 | 0.23 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 8 | 0.23 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 4 | 0.23 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 6 | 0.23 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 2 | 0.23 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 10 | 0.23 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 3 | 0.23 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 1 | 0.23 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 3 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 5 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 7 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 7 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 7 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 7 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 7 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 7 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 7 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 7 | 0.23 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 7 | 0.23 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 1 | 0.23 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 1 | 0.23 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 8 | 0.23 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 8 | 0.23 |
| (2,327) | 2:B:162:LEU:H | 2:B:162:LEU:HB2 | 5 | 0.23 |
| (2,327) | 2:B:162:LEU:H | 2:B:162:LEU:HB3 | 5 | 0.23 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 5 | 0.23 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 5 | 0.23 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 6 | 0.23 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 6 | 0.23 |
| (2,325) | 2:B:161:LYS:H | 2:B:161:LYS:HB2 | 2 | 0.23 |
| (2,325) | 2:B:161:LYS:H | 2:B:161:LYS:HB3 | 2 | 0.23 |
| (2,325) | 2:B:161:LYS:H | 2:B:161:LYS:HB2 | 8 | 0.23 |
| (2,325) | 2:B:161:LYS:H | 2:B:161:LYS:HB3 | 8 | 0.23 |
| (2,3247) | 2:B:162:LEU:H | 2:B:162:LEU:HB2 | 5 | 0.23 |
| (2,3247) | 2:B:162:LEU:H | 2:B:162:LEU:HB3 | 5 | 0.23 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 4 | 0.23 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 4 | 0.23 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 4 | 0.23 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 4 | 0.23 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 4 | 0.23 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 7 | 0.23 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 7 | 0.23 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 7 | 0.23 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 4 | 0.23 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 4 | 0.23 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 9 | 0.23 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 9 | 0.23 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 9 | 0.23 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 9 | 0.23 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 9 | 0.23 |
| (2,3025) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HE2 | 6 | 0.23 |
| (2,3025) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HE3 | 6 | 0.23 |
| (2,3025) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HE2 | 6 | 0.23 |
| (2,3025) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HE3 | 6 | 0.23 |
| (2,3025) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HE2 | 6 | 0.23 |
| (2,3025) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HE3 | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 7 | 0.23 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 7 | 0.23 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 7 | 0.23 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 7 | 0.23 |
| (2,3021) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 7 | 0.23 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 3 | 0.23 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 3 | 0.23 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 4 | 0.23 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 4 | 0.23 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 4 | 0.23 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 5 | 0.23 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 5 | 0.23 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 7 | 0.23 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 7 | 0.23 |
| (2,2703) | 2:B:109:LEU:HD12 | 2:B:109:LEU:H | 8 | 0.23 |
| (2,2703) | 2:B:109:LEU:HD13 | 2:B:109:LEU:H | 8 | 0.23 |
| (2,2703) | 2:B:109:LEU:HD22 | 2:B:109:LEU:H | 8 | 0.23 |
| (2,2703) | 2:B:109:LEU:HD21 | 2:B:109:LEU:H | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 1 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 2 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 3 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 4 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 5 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 6 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 7 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 8 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 9 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2689) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 10 | 0.23 |
| (2,2689) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 10 | 0.23 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 3 | 0.23 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 3 | 0.23 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 3 | 0.23 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 3 | 0.23 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 3 | 0.23 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 3 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 2 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 2 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 2 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 2 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 2 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 2 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 10 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 10 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 10 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 10 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 10 | 0.23 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 10 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG22 | 4 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG21 | 4 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG22 | 4 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG21 | 4 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG23 | 4 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HD12 | 4 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG22 | 4 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG21 | 4 | 0.23 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG23 | 4 | 0.23 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 4 | 0.23 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 4 | 0.23 |
| (2,2328) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 4 | 0.23 |
| (2,2286) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 3 | 0.23 |
| (2,2286) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 3 | 0.23 |
| (2,2285) | 1:A:28:ILE:HA | 1:A:31:LEU:HD22 | 10 | 0.23 |
| (2,2285) | 1:A:28:ILE:HA | 1:A:31:LEU:HD11 | 10 | 0.23 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 8 | 0.23 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 8 | 0.23 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 8 | 0.23 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 6 | 0.23 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 6 | 0.23 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 6 | 0.23 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 2 | 0.23 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 2 | 0.23 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 9 | 0.23 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 9 | 0.23 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 9 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 10 | 0.23 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 10 | 0.23 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 2 | 0.23 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 2 | 0.23 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 2 | 0.23 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 2 | 0.23 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 2 | 0.23 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 2 | 0.23 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 2 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 1 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 1 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 1 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 1 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 4 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 4 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 4 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 4 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 5 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 5 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 5 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 5 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 6 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 6 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 6 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 6 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 10 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 10 | 0.23 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 10 | 0.23 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 1 | 0.23 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 1 | 0.23 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 1 | 0.23 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 9 | 0.23 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 9 | 0.23 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 10 | 0.23 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 10 | 0.23 |
| (2,1614) | 2:B:101:MET:HE1 | 1:A:14:LEU:HB2 | 8 | 0.23 |
| (2,1614) | 2:B:101:MET:HE3 | 1:A:14:LEU:HB2 | 8 | 0.23 |
| (2,1614) | 2:B:101:MET:HE2 | 1:A:14:LEU:HB2 | 8 | 0.23 |
| (2,159) | 1:A:63:VAL:H | 1:A:62:ASN:HB2 | 1 | 0.23 |
| (2,159) | 1:A:63:VAL:H | 1:A:62:ASN:HB3 | 1 | 0.23 |
| (2,1510) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 3 | 0.23 |
| (2,1510) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 3 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD12 | 1:A:56:ILE:HD12 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD12 | 1:A:56:ILE:HD11 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD12 | 1:A:56:ILE:HD13 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD11 | 1:A:56:ILE:HD12 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD11 | 1:A:56:ILE:HD11 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD11 | 1:A:56:ILE:HD13 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD13 | 1:A:56:ILE:HD12 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD13 | 1:A:56:ILE:HD11 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD13 | 1:A:56:ILE:HD13 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD21 | 1:A:56:ILE:HD12 | 4 | 0.23 |
| (2,1334) | 1:A:14:LEU:HD21 | 1:A:56:ILE:HD11 | 4 | 0.23 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 2 | 0.23 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 2 | 0.23 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 2 | 0.23 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 2 | 0.23 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 10 | 0.23 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 10 | 0.23 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 10 | 0.23 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD2 | 9 | 0.23 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD3 | 9 | 0.23 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 3 | 0.23 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 3 | 0.23 |
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 1 | 0.23 |
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 1 | 0.23 |
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 1 | 0.23 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 9 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 9 | 0.23 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 9 | 0.23 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 6 | 0.23 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 6 | 0.23 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 5 | 0.23 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 5 | 0.23 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 5 | 0.23 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 1 | 0.23 |
| (1,83) | 2:B:139:LEU:N | 2:B:135:ASP:O | 4 | 0.23 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 5 | 0.23 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 6 | 0.23 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 9 | 0.23 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 7 | 0.22 |
| (2,958) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 7 | 0.22 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 6 | 0.22 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 6 | 0.22 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 2 | 0.22 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 2 | 0.22 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 2 | 0.22 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 2 | 0.22 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 3 | 0.22 |
| (2,787) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 3 | 0.22 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 6 | 0.22 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 6 | 0.22 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 10 | 0.22 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 10 | 0.22 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 10 | 0.22 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 6 | 0.22 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 6 | 0.22 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 6 | 0.22 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 6 | 0.22 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 6 | 0.22 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 6 | 0.22 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 6 | 0.22 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 6 | 0.22 |
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG12 | 2:B:112:LEU:HD23 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD22 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD21 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 6 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD21 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 6 | 0.22 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 6 | 0.22 |
| (2,502) | 1:A:26:ASP:HB2 | 1:A:30:ALA:HB2 | 9 | 0.22 |
| (2,502) | 1:A:26:ASP:HB2 | 1:A:30:ALA:HB1 | 9 | 0.22 |
| (2,502) | 1:A:26:ASP:HB2 | 1:A:30:ALA:HB3 | 9 | 0.22 |
| (2,502) | 1:A:26:ASP:HB3 | 1:A:30:ALA:HB2 | 9 | 0.22 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 5 | 0.22 |
| (2,4556) | 2:B:161:LYS:HA | 2:B:161:LYS:H | 6 | 0.22 |
| (2,4509) | 2:B:142:VAL:HB | 2:B:143:ILE:H | 5 | 0.22 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 4 | 0.22 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 8 | 0.22 |
| (2,4149) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 9 | 0.22 |
| (2,4119) | 2:B:155:ILE:HB | 2:B:152:GLU:HA | 7 | 0.22 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG12 | 9 | 0.22 |
| (2,4090) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 9 | 0.22 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 1 | 0.22 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 8 | 0.22 |
| (2,3999) | 2:B:160:GLY:H | 2:B:162:LEU:H | 2 | 0.22 |
| (2,3999) | 2:B:160:GLY:H | 2:B:162:LEU:H | 8 | 0.22 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 2 | 0.22 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 2 | 0.22 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 2 | 0.22 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 3 | 0.22 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 3 | 0.22 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 3 | 0.22 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 5 | 0.22 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 5 | 0.22 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 5 | 0.22 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 7 | 0.22 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 7 | 0.22 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 7 | 0.22 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 1 | 0.22 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 1 | 0.22 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 5 | 0.22 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 5 | 0.22 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 7 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 2 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 2 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 2 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 2 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 2 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 2 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 2 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 2 | 0.22 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 2 | 0.22 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 2 | 0.22 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 2 | 0.22 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 2 | 0.22 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 2 | 0.22 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 2 | 0.22 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 2 | 0.22 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 2 | 0.22 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 2 | 0.22 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 3 | 0.22 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 3 | 0.22 |
| (2,327) | 2:B:162:LEU:H | 2:B:162:LEU:HB2 | 9 | 0.22 |
| (2,327) | 2:B:162:LEU:H | 2:B:162:LEU:HB3 | 9 | 0.22 |
| (2,3247) | 2:B:162:LEU:H | 2:B:162:LEU:HB2 | 9 | 0.22 |
| (2,3247) | 2:B:162:LEU:H | 2:B:162:LEU:HB3 | 9 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 10 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 10 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 10 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 10 | 0.22 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 10 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 8 | 0.22 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 8 | 0.22 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 2 | 0.22 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 2 | 0.22 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 2 | 0.22 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 6 | 0.22 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 6 | 0.22 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG21 | 3 | 0.22 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG23 | 3 | 0.22 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 10 | 0.22 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 10 | 0.22 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 10 | 0.22 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 10 | 0.22 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 3 | 0.22 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 3 | 0.22 |
| (2,2979) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 3 | 0.22 |
| (2,2979) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 3 | 0.22 |
| (2,2916) | 2:B:128:ASP:HB2 | 2:B:124:LYS:HB2 | 5 | 0.22 |
| (2,2916) | 2:B:128:ASP:HB2 | 2:B:124:LYS:HB3 | 5 | 0.22 |
| (2,2916) | 2:B:128:ASP:HB2 | 2:B:125:LYS:HB3 | 5 | 0.22 |
| (2,2916) | 2:B:128:ASP:HB3 | 2:B:124:LYS:HB2 | 5 | 0.22 |
| (2,2916) | 2:B:128:ASP:HB3 | 2:B:124:LYS:HB3 | 5 | 0.22 |
| (2,2916) | 2:B:128:ASP:HB3 | 2:B:125:LYS:HB3 | 5 | 0.22 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG3 | 7 | 0.22 |
| (2,2878) | 2:B:126:ILE:HA | 2:B:125:LYS:HG2 | 7 | 0.22 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 8 | 0.22 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 8 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD12 | 2:B:109:LEU:H | 5 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD13 | 2:B:109:LEU:H | 5 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD22 | 2:B:109:LEU:H | 5 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD21 | 2:B:109:LEU:H | 5 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD12 | 2:B:109:LEU:H | 6 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD13 | 2:B:109:LEU:H | 6 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD22 | 2:B:109:LEU:H | 6 | 0.22 |
| (2,2703) | 2:B:109:LEU:HD21 | 2:B:109:LEU:H | 6 | 0.22 |
| (2,266) | 2:B:134:ALA:H | 2:B:133:GLU:HG2 | 3 | 0.22 |
| (2,266) | 2:B:134:ALA:H | 2:B:133:GLU:HG3 | 3 | 0.22 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 10 | 0.22 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 10 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG12 | 8 | 0.22 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG11 | 8 | 0.22 |
| (2,2416) | 1:A:40:GLU:HG2 | 1:A:39:VAL:HG13 | 8 | 0.22 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG12 | 8 | 0.22 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG11 | 8 | 0.22 |
| (2,2416) | 1:A:40:GLU:HG3 | 1:A:39:VAL:HG13 | 8 | 0.22 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 5 | 0.22 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 5 | 0.22 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 5 | 0.22 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 5 | 0.22 |
| (2,2267) | 1:A:26:ASP:HB2 | 1:A:30:ALA:HB2 | 9 | 0.22 |
| (2,2267) | 1:A:26:ASP:HB2 | 1:A:30:ALA:HB1 | 9 | 0.22 |
| (2,2267) | 1:A:26:ASP:HB2 | 1:A:30:ALA:HB3 | 9 | 0.22 |
| (2,2267) | 1:A:26:ASP:HB3 | 1:A:30:ALA:HB2 | 9 | 0.22 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG22 | 5 | 0.22 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG21 | 5 | 0.22 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG23 | 5 | 0.22 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD21 | 5 | 0.22 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD23 | 5 | 0.22 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG22 | 5 | 0.22 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG21 | 5 | 0.22 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG23 | 5 | 0.22 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 2 | 0.22 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 2 | 0.22 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 2 | 0.22 |
| (2,2094) | 1:A:10:ILE:HD11 | 1:A:7:LEU:H | 8 | 0.22 |
| (2,2094) | 1:A:10:ILE:HD13 | 1:A:7:LEU:H | 8 | 0.22 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 10 | 0.22 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 10 | 0.22 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 3 | 0.22 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 3 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 5 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 5 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 9 | 0.22 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 9 | 0.22 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 1 | 0.22 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 1 | 0.22 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 7 | 0.22 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 7 | 0.22 |
| (2,1860) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 7 | 0.22 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 5 | 0.22 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 5 | 0.22 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 5 | 0.22 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 2 | 0.22 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 2 | 0.22 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 4 | 0.22 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 4 | 0.22 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 7 | 0.22 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 7 | 0.22 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 8 | 0.22 |
| (2,1708) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 8 | 0.22 |
| (2,1654) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 4 | 0.22 |
| (2,1654) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 4 | 0.22 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 4 | 0.22 |
| (2,1654) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 4 | 0.22 |
| (2,1272) | 1:A:2:ALA:HB2 | 1:A:6:GLU:HB3 | 3 | 0.22 |
| (2,1272) | 1:A:2:ALA:HB1 | 1:A:6:GLU:HB3 | 3 | 0.22 |
| (2,1272) | 1:A:2:ALA:HB3 | 1:A:6:GLU:HB3 | 3 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1198) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 8 | 0.22 |
| (2,1198) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 8 | 0.22 |
| (2,1198) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 8 | 0.22 |
| (2,1198) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 8 | 0.22 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 3 | 0.22 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 3 | 0.22 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 7 | 0.22 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 7 | 0.22 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 4 | 0.22 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 4 | 0.22 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD11 | 10 | 0.22 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD13 | 10 | 0.22 |
| (2,1132) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 10 | 0.22 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD21 | 10 | 0.22 |
| (2,1132) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 10 | 0.22 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD12 | 10 | 0.22 |
| (2,1132) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 10 | 0.22 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 1 | 0.22 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 1 | 0.22 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 1 | 0.22 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 3 | 0.22 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 3 | 0.22 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 3 | 0.22 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 2 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 2 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 4 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 4 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 7 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 7 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 8 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 8 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 9 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 9 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 10 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 10 | 0.21 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 2 | 0.21 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 2 | 0.21 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 7 | 0.21 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 7 | 0.21 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 8 | 0.21 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 8 | 0.21 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 10 | 0.21 |
| (2,761) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 3 | 0.21 |
| (2,761) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 3 | 0.21 |
| (2,761) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 3 | 0.21 |
| (2,739) | 1:A:59:LEU:HD12 | 1:A:56:ILE:HA | 6 | 0.21 |
| (2,739) | 1:A:59:LEU:HD11 | 1:A:56:ILE:HA | 6 | 0.21 |
| (2,739) | 1:A:59:LEU:HD13 | 1:A:56:ILE:HA | 6 | 0.21 |
| (2,739) | 1:A:59:LEU:HD21 | 1:A:56:ILE:HA | 6 | 0.21 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 8 | 0.21 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 8 | 0.21 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 8 | 0.21 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 8 | 0.21 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 8 | 0.21 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 8 | 0.21 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 8 | 0.21 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 8 | 0.21 |
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 8 | 0.21 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG2 | 4 | 0.21 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG3 | 4 | 0.21 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG2 | 9 | 0.21 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG3 | 9 | 0.21 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 6 | 0.21 |
| (2,4538) | 2:B:152:GLU:H | 2:B:152:GLU:HG2 | 6 | 0.21 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 6 | 0.21 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 1 | 0.21 |
| (2,4517) | 2:B:144:SER:HA | 2:B:143:ILE:HB | 3 | 0.21 |
| (2,4456) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 6 | 0.21 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 1 | 0.21 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 1 | 0.21 |
| (2,4164) | 1:A:59:LEU:HB3 | 1:A:59:LEU:HG | 6 | 0.21 |
| (2,4119) | 2:B:155:ILE:HB | 2:B:152:GLU:HA | 8 | 0.21 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 4 | 0.21 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 4 | 0.21 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 4 | 0.21 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 6 | 0.21 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 6 | 0.21 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 6 | 0.21 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 9 | 0.21 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 4 | 0.21 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG22 | 2 | 0.21 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG21 | 2 | 0.21 |
| (2,3506) | 1:A:60:ILE:HB | 2:B:159:ILE:HG23 | 2 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 10 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 10 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 10 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 10 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 10 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 10 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 10 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 10 | 0.21 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 10 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 8 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 8 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 8 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 8 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 8 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 8 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 8 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 8 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 10 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 10 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 10 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 10 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 10 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 10 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 10 | 0.21 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 10 | 0.21 |
| (2,3416) | 2:B:101:MET:HE2 | 1:A:17:HIS:HD2 | 8 | 0.21 |
| (2,3416) | 2:B:101:MET:HE1 | 1:A:17:HIS:HD2 | 8 | 0.21 |
| (2,3416) | 2:B:101:MET:HE3 | 1:A:17:HIS:HD2 | 8 | 0.21 |
| (2,3342) | 1:A:15:ILE:HD11 | 2:B:106:SER:HA | 4 | 0.21 |
| (2,3342) | 1:A:15:ILE:HD13 | 2:B:106:SER:HA | 4 | 0.21 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 4 | 0.21 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 4 | 0.21 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 10 | 0.21 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 10 | 0.21 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 10 | 0.21 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 10 | 0.21 |
| (2,325) | 2:B:161:LYS:H | 2:B:161:LYS:HB2 | 1 | 0.21 |
| (2,325) | 2:B:161:LYS:H | 2:B:161:LYS:HB3 | 1 | 0.21 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG2 | 3 | 0.21 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG3 | 3 | 0.21 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 10 | 0.21 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 10 | 0.21 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 10 | 0.21 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 10 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 5 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 5 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 5 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 6 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 6 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 6 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 9 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 9 | 0.21 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 9 | 0.21 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG22 | 3 | 0.21 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG21 | 3 | 0.21 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG21 | 3 | 0.21 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG23 | 3 | 0.21 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD12 | 3 | 0.21 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD11 | 3 | 0.21 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD13 | 3 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 2 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 2 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 2 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 6 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 6 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 6 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 9 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 9 | 0.21 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 9 | 0.21 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 1 | 0.21 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 1 | 0.21 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 1 | 0.21 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 1 | 0.21 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 3 | 0.21 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 3 | 0.21 |
| (2,2627) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 3 | 0.21 |
| (2,2627) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 3 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 1 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 1 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 2 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 2 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 3 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 3 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 4 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 4 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 5 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 5 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 6 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 6 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 7 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 7 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 8 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 8 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 9 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 9 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 10 | 0.21 |
| (2,2442) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 10 | 0.21 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 10 | 0.21 |
| (2,2339) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 10 | 0.21 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG2 | 10 | 0.21 |
| (2,2337) | 1:A:33:LYS:H | 1:A:33:LYS:HG3 | 10 | 0.21 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 1 | 0.21 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 1 | 0.21 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 1 | 0.21 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 1 | 0.21 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 7 | 0.21 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 7 | 0.21 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 7 | 0.21 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 7 | 0.21 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 1 | 0.21 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 1 | 0.21 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 1 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 1 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 1 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 1 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 1 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 1 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 2 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 2 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 2 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 2 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 2 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 3 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 3 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 3 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 3 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 3 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 4 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 4 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 4 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 4 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 4 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 5 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 5 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 5 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 5 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 5 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 6 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 6 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 6 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 6 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 6 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 7 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 7 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 7 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 7 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 7 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 8 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 8 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 8 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 8 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 8 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD12 | 9 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD13 | 9 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD22 | 9 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD21 | 9 | 0.21 |
| (2,2140) | 1:A:14:LEU:HG | 1:A:14:LEU:HD23 | 9 | 0.21 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 9 | 0.21 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 9 | 0.21 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 9 | 0.21 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 5 | 0.21 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 5 | 0.21 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 6 | 0.21 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 6 | 0.21 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 8 | 0.21 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 8 | 0.21 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 9 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 9 | 0.21 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 2 | 0.21 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 1 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 2 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 4 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 6 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 6 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 7 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 8 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD12 | 2:B:162:LEU:HD11 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD11 | 2:B:162:LEU:HD13 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD21 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD22 | 2:B:162:LEU:HD23 | 10 | 0.21 |
| (2,2003) | 2:B:162:LEU:HD21 | 2:B:162:LEU:HD23 | 10 | 0.21 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG22 | 2 | 0.21 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG21 | 2 | 0.21 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG23 | 2 | 0.21 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG12 | 2 | 0.21 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG11 | 2 | 0.21 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG22 | 2 | 0.21 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG21 | 2 | 0.21 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG23 | 2 | 0.21 |
| (2,1989) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 9 | 0.21 |
| (2,1989) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 9 | 0.21 |
| (2,1967) | 2:B:157:GLN:HA | 2:B:157:GLN:HG2 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1967) | 2:B:157:GLN:HA | 2:B:157:GLN:HG3 | 10 | 0.21 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 10 | 0.21 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 10 | 0.21 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 10 | 0.21 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 10 | 0.21 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 9 | 0.21 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 9 | 0.21 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 9 | 0.21 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 9 | 0.21 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 7 | 0.21 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 7 | 0.21 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 7 | 0.21 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 7 | 0.21 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 7 | 0.21 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 3 | 0.21 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 3 | 0.21 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 3 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 3 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 3 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 3 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 3 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 5 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 5 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 5 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 5 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 7 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 7 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 7 | 0.21 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 7 | 0.21 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 2 | 0.21 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 2 | 0.21 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 1 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 2 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 5 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 6 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 8 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 9 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 9 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 9 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 9 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 9 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 9 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 9 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 9 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 9 | 0.21 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 9 | 0.21 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 6 | 0.21 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 6 | 0.21 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 9 | 0.21 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 9 | 0.21 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 2 | 0.21 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 2 | 0.21 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 4 | 0.21 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 4 | 0.21 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 7 | 0.21 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 7 | 0.21 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 10 | 0.21 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 10 | 0.21 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 7 | 0.21 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 7 | 0.21 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 7 | 0.21 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 9 | 0.21 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 9 | 0.21 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 9 | 0.21 |
| (2,1034) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 8 | 0.21 |
| (2,1034) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 8 | 0.21 |
| (2,1034) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 8 | 0.21 |
| (2,1034) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 8 | 0.21 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 9 | 0.21 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 10 | 0.21 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 4 | 0.21 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 8 | 0.21 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 1 | 0.2 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 1 | 0.2 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 3 | 0.2 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 3 | 0.2 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 5 | 0.2 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 5 | 0.2 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 6 | 0.2 |
| (2,860) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 6 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 9 | 0.2 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 9 | 0.2 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE2 | 2 | 0.2 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE1 | 2 | 0.2 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE3 | 2 | 0.2 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 6 | 0.2 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 6 | 0.2 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 6 | 0.2 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 6 | 0.2 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 6 | 0.2 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB2 | 9 | 0.2 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB3 | 9 | 0.2 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 4 | 0.2 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 4 | 0.2 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 4 | 0.2 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 4 | 0.2 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 4 | 0.2 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 4 | 0.2 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 4 | 0.2 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 4 | 0.2 |
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 4 | 0.2 |
| (2,587) | 1:A:37:VAL:HG12 | 2:B:112:LEU:HD23 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD22 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD21 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD21 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 9 | 0.2 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 9 | 0.2 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 9 | 0.2 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 10 | 0.2 |
| (2,4509) | 2:B:142:VAL:HB | 2:B:143:ILE:H | 9 | 0.2 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 3 | 0.2 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 6 | 0.2 |
| (2,4393) | 1:A:63:VAL:HA | 1:A:64:GLY:H | 5 | 0.2 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 5 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 10 | 0.2 |
| (2,4251) | 1:A:15:ILE:HA | 2:B:103:TYR:HA | 3 | 0.2 |
| (2,4119) | 2:B:155:ILE:HB | 2:B:152:GLU:HA | 6 | 0.2 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 5 | 0.2 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 6 | 0.2 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 4 | 0.2 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 1 | 0.2 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 1 | 0.2 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 1 | 0.2 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 10 | 0.2 |
| (2,3840) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 1 | 0.2 |
| (2,3840) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 5 | 0.2 |
| (2,3840) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 8 | 0.2 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 3 | 0.2 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 1 | 0.2 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 8 | 0.2 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 9 | 0.2 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 8 | 0.2 |
| (2,3596) | 1:A:21:VAL:H | 1:A:22:THR:H | 9 | 0.2 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 8 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 1 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 1 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 1 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 1 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 1 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 1 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 1 | 0.2 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 1 | 0.2 |
| (2,3430) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 5 | 0.2 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 5 | 0.2 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 5 | 0.2 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB2 | 1 | 0.2 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB3 | 1 | 0.2 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB2 | 1 | 0.2 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB3 | 1 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG22 | 2:B:101:MET:HE2 | 4 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE2 | 4 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE3 | 4 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE2 | 4 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE1 | 4 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE3 | 4 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG22 | 2:B:101:MET:HE2 | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE2 | 9 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE3 | 9 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE2 | 9 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE1 | 9 | 0.2 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE3 | 9 | 0.2 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 10 | 0.2 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 10 | 0.2 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 10 | 0.2 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 10 | 0.2 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 10 | 0.2 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 10 | 0.2 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 2 | 0.2 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 2 | 0.2 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 6 | 0.2 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 6 | 0.2 |
| (2,327) | 2:B:162:LEU:H | 2:B:162:LEU:HB2 | 3 | 0.2 |
| (2,327) | 2:B:162:LEU:H | 2:B:162:LEU:HB3 | 3 | 0.2 |
| (2,3247) | 2:B:162:LEU:H | 2:B:162:LEU:HB2 | 3 | 0.2 |
| (2,3247) | 2:B:162:LEU:H | 2:B:162:LEU:HB3 | 3 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 5 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 5 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 5 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 5 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 5 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 7 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 7 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 7 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 7 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 7 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 9 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 9 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 9 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 9 | 0.2 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 9 | 0.2 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 9 | 0.2 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 9 | 0.2 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 9 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 1 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 1 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 1 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 4 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 4 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 4 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 8 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 8 | 0.2 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 8 | 0.2 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 10 | 0.2 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 10 | 0.2 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 5 | 0.2 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.2 |
| (2,3102) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.2 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD12 | 1 | 0.2 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD11 | 1 | 0.2 |
| (2,3069) | 2:B:143:ILE:H | 2:B:143:ILE:HD13 | 1 | 0.2 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 2 | 0.2 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 2 | 0.2 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 2 | 0.2 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 9 | 0.2 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 9 | 0.2 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 9 | 0.2 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 9 | 0.2 |
| (2,3010) | 2:B:138:ARG:HG2 | 2:B:135:ASP:H | 10 | 0.2 |
| (2,3010) | 2:B:138:ARG:HG3 | 2:B:135:ASP:H | 10 | 0.2 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 2 | 0.2 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 2 | 0.2 |
| (2,2979) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 2 | 0.2 |
| (2,2979) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 2 | 0.2 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 9 | 0.2 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 9 | 0.2 |
| (2,2810) | 2:B:119:SER:HB2 | 2:B:120:ALA:HB2 | 4 | 0.2 |
| (2,2810) | 2:B:119:SER:HB2 | 2:B:120:ALA:HB1 | 4 | 0.2 |
| (2,2810) | 2:B:119:SER:HB2 | 2:B:120:ALA:HB3 | 4 | 0.2 |
| (2,2810) | 2:B:119:SER:HB2 | 2:B:121:LYS:HG2 | 4 | 0.2 |
| (2,2810) | 2:B:119:SER:HB3 | 2:B:118:PRO:HB2 | 4 | 0.2 |
| (2,2810) | 2:B:119:SER:HB3 | 2:B:118:PRO:HB3 | 4 | 0.2 |
| (2,2810) | 2:B:119:SER:HB3 | 2:B:120:ALA:HB2 | 4 | 0.2 |
| (2,2810) | 2:B:119:SER:HB3 | 2:B:120:ALA:HB1 | 4 | 0.2 |
| (2,2810) | 2:B:119:SER:HB3 | 2:B:121:LYS:HG2 | 4 | 0.2 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 6 | 0.2 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 6 | 0.2 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 1 | 0.2 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 1 | 0.2 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 5 | 0.2 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 5 | 0.2 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 5 | 0.2 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 5 | 0.2 |
| (2,2328) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 5 | 0.2 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 1 | 0.2 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 1 | 0.2 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 4 | 0.2 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 4 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 8 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 8 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 8 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 8 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 10 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 10 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 10 | 0.2 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 10 | 0.2 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 5 | 0.2 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 5 | 0.2 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 5 | 0.2 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 8 | 0.2 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 8 | 0.2 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 8 | 0.2 |
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 8 | 0.2 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 4 | 0.2 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 4 | 0.2 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 5 | 0.2 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 5 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 7 | 0.2 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 7 | 0.2 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG22 | 6 | 0.2 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG21 | 6 | 0.2 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:165:VAL:HG23 | 6 | 0.2 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG12 | 6 | 0.2 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG11 | 6 | 0.2 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG22 | 6 | 0.2 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG21 | 6 | 0.2 |
| (2,1996) | 2:B:162:LEU:HA | 2:B:104:VAL:HG23 | 6 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 1 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 8 | 0.2 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 8 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG12 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG13 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD2 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD3 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG12 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG13 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HD3 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:151:ILE:HG12 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HD3 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG12 | 6 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG13 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:155:ILE:HG12 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG12 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG13 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HD3 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG12 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG13 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HD3 | 6 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG12 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG13 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD2 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD3 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG12 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG13 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HD3 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:151:ILE:HG12 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HD3 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG12 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG13 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:155:ILE:HG12 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG12 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG13 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HD3 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG12 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG13 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HD3 | 7 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG12 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG13 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD2 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD3 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG12 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG13 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HD3 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:151:ILE:HG12 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HD3 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG12 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG13 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:155:ILE:HG12 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG12 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG13 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HD3 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG12 | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG13 | 9 | 0.2 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HD3 | 9 | 0.2 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG2 | 1 | 0.2 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG3 | 1 | 0.2 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG2 | 9 | 0.2 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG3 | 9 | 0.2 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 7 | 0.2 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 7 | 0.2 |
| (2,1862) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 7 | 0.2 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 9 | 0.2 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 9 | 0.2 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 9 | 0.2 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 9 | 0.2 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 9 | 0.2 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 5 | 0.2 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 5 | 0.2 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG12 | 7 | 0.2 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG11 | 7 | 0.2 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG13 | 7 | 0.2 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG22 | 7 | 0.2 |
| (2,160) | 1:A:64:GLY:H | 1:A:63:VAL:HG23 | 7 | 0.2 |
| (2,158) | 1:A:63:VAL:H | 1:A:63:VAL:HG23 | 1 | 0.2 |
| (2,158) | 1:A:63:VAL:H | 1:A:63:VAL:HG12 | 1 | 0.2 |
| (2,158) | 1:A:63:VAL:H | 1:A:63:VAL:HG11 | 1 | 0.2 |
| (2,158) | 1:A:63:VAL:H | 1:A:63:VAL:HG13 | 1 | 0.2 |
| (2,158) | 1:A:63:VAL:H | 1:A:63:VAL:HG22 | 1 | 0.2 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 2 | 0.2 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 2 | 0.2 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 2 | 0.2 |
| (2,1391) | 1:A:24:THR:HG21 | 1:A:27:LYS:HE3 | 5 | 0.2 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE2 | 5 | 0.2 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE3 | 5 | 0.2 |
| (2,1391) | 1:A:24:THR:HG23 | 1:A:27:LYS:HE3 | 5 | 0.2 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 2 | 0.2 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 2 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 3 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 4 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 7 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG11 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG12 | 1:A:4:VAL:HG13 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG11 | 1:A:4:VAL:HG13 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG22 | 1:A:4:VAL:HG21 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 10 | 0.2 |
| (2,1286) | 1:A:4:VAL:HG21 | 1:A:4:VAL:HG23 | 10 | 0.2 |
| (2,1219) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 9 | 0.2 |
| (2,1219) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 9 | 0.2 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 9 | 0.2 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 9 | 0.2 |
| (2,1194) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 8 | 0.2 |
| (2,1194) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 8 | 0.2 |
| (2,1194) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 8 | 0.2 |
| (2,1194) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 8 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 1 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 2 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 2 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 4 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 4 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 5 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 5 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 8 | 0.2 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 1 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 2 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 3 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 4 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 4 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 5 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 6 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 7 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 8 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 9 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD12 | 2:B:146:LEU:HD13 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD11 | 2:B:146:LEU:HD13 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD21 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD22 | 2:B:146:LEU:HD23 | 10 | 0.2 |
| (2,1126) | 2:B:146:LEU:HD21 | 2:B:146:LEU:HD23 | 10 | 0.2 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 2 | 0.2 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 2 | 0.2 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 2 | 0.2 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG2 | 2 | 0.2 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG3 | 2 | 0.2 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 1 | 0.2 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 5 | 0.19 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 5 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 1 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 1 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 2 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 2 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 3 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 3 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 4 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 4 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 5 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 5 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 6 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 6 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 7 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 7 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 8 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 8 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 9 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 9 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 10 | 0.19 |
| (2,816) | 2:B:107:TYR:HB2 | 2:B:107:TYR:HB3 | 10 | 0.19 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 2 | 0.19 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 2 | 0.19 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 6 | 0.19 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 6 | 0.19 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 7 | 0.19 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 7 | 0.19 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD13 | 2 | 0.19 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD22 | 2 | 0.19 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD21 | 2 | 0.19 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD23 | 2 | 0.19 |
| (2,628) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 8 | 0.19 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 8 | 0.19 |
| (2,628) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 8 | 0.19 |
| (2,586) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 1 | 0.19 |
| (2,586) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 1 | 0.19 |
| (2,586) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 1 | 0.19 |
| (2,586) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 1 | 0.19 |
| (2,586) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 1 | 0.19 |
| (2,569) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 4 | 0.19 |
| (2,569) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,569) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 6 | 0.19 |
| (2,569) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,569) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 8 | 0.19 |
| (2,569) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,569) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 9 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 9 | 0.19 |
| (2,569) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 9 | 0.19 |
| (2,569) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 9 | 0.19 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG2 | 1 | 0.19 |
| (2,458) | 1:A:20:GLU:HA | 1:A:20:GLU:HG3 | 1 | 0.19 |
| (2,4556) | 2:B:161:LYS:HA | 2:B:161:LYS:H | 3 | 0.19 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 9 | 0.19 |
| (2,4509) | 2:B:142:VAL:HB | 2:B:143:ILE:H | 2 | 0.19 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 4 | 0.19 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 7 | 0.19 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 8 | 0.19 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 9 | 0.19 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 3 | 0.19 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 8 | 0.19 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 4 | 0.19 |
| (2,4183) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 3 | 0.19 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 5 | 0.19 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 7 | 0.19 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 10 | 0.19 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 7 | 0.19 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 7 | 0.19 |
| (2,389) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 10 | 0.19 |
| (2,389) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 10 | 0.19 |
| (2,389) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 10 | 0.19 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 2 | 0.19 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 1 | 0.19 |
| (2,3840) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 2 | 0.19 |
| (2,3840) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 3 | 0.19 |
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 2 | 0.19 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 9 | 0.19 |
| (2,3769) | 2:B:106:SER:H | 2:B:104:VAL:HB | 5 | 0.19 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 1 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 4 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 4 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 4 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 4 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 4 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 4 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 4 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 4 | 0.19 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 4 | 0.19 |
| (2,3492) | 2:B:152:GLU:HG2 | 1:A:7:LEU:HB3 | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB2 | 1 | 0.19 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB3 | 1 | 0.19 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 4 | 0.19 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 4 | 0.19 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 4 | 0.19 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 4 | 0.19 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 4 | 0.19 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 4 | 0.19 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 4 | 0.19 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 4 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD12 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD11 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD13 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:109:LEU:HD13 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD12 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD11 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD13 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD12 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD11 | 10 | 0.19 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD13 | 10 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 4 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 6 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 8 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 9 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 9 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 9 | 0.19 |
| (2,3373) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 9 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 4 | 0.19 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 4 | 0.19 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 10 | 0.19 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 10 | 0.19 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 4 | 0.19 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 4 | 0.19 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG2 | 7 | 0.19 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG3 | 7 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 3 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 3 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 3 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 5 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 5 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 5 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 6 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 6 | 0.19 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 6 | 0.19 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 8 | 0.19 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 8 | 0.19 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 8 | 0.19 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 8 | 0.19 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 8 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 3 | 0.19 |
| (2,3177) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 3 | 0.19 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 2 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 2 | 0.19 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 2 | 0.19 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 4 | 0.19 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 4 | 0.19 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 8 | 0.19 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 8 | 0.19 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 2 | 0.19 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 2 | 0.19 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 2 | 0.19 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 2 | 0.19 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 1 | 0.19 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 1 | 0.19 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 4 | 0.19 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 4 | 0.19 |
| (2,3054) | 2:B:142:VAL:HG12 | 2:B:107:TYR:HD2 | 3 | 0.19 |
| (2,3054) | 2:B:142:VAL:HG11 | 2:B:107:TYR:HD2 | 3 | 0.19 |
| (2,3054) | 2:B:142:VAL:HG13 | 2:B:107:TYR:HD2 | 3 | 0.19 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD1 | 3 | 0.19 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD2 | 3 | 0.19 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HE2 | 3 | 0.19 |
| (2,3054) | 2:B:142:VAL:HG21 | 2:B:107:TYR:HD2 | 3 | 0.19 |
| (2,3054) | 2:B:142:VAL:HG23 | 2:B:107:TYR:HD2 | 3 | 0.19 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 9 | 0.19 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 9 | 0.19 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 9 | 0.19 |
| (2,2860) | 2:B:124:LYS:HG2 | 2:B:124:LYS:HE3 | 5 | 0.19 |
| (2,2860) | 2:B:124:LYS:HG3 | 2:B:124:LYS:HE3 | 5 | 0.19 |
| (2,2860) | 2:B:124:LYS:HG3 | 2:B:124:LYS:HE2 | 5 | 0.19 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 7 | 0.19 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 7 | 0.19 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 7 | 0.19 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 7 | 0.19 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 7 | 0.19 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 7 | 0.19 |
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 7 | 0.19 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 1 | 0.19 |
| (2,2639) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 1 | 0.19 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 7 | 0.19 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 7 | 0.19 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 5 | 0.19 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 5 | 0.19 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG2 | 10 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG3 | 10 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 4 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 4 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 6 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 6 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 8 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 8 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB2 | 2:B:125:LYS:HE2 | 9 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE2 | 9 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB1 | 2:B:125:LYS:HE3 | 9 | 0.19 |
| (2,2341) | 1:A:34:ALA:HB3 | 2:B:125:LYS:HE2 | 9 | 0.19 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 3 | 0.19 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 3 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 2 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 2 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 2 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 2 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 3 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 3 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 3 | 0.19 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 3 | 0.19 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 3 | 0.19 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 3 | 0.19 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 3 | 0.19 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 7 | 0.19 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 7 | 0.19 |
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 7 | 0.19 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 8 | 0.19 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 8 | 0.19 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 8 | 0.19 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 3 | 0.19 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 3 | 0.19 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 1 | 0.19 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 1 | 0.19 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 6 | 0.19 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 6 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 6 | 0.19 |
| (2,1989) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 6 | 0.19 |
| (2,1989) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 6 | 0.19 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 2 | 0.19 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 2 | 0.19 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 10 | 0.19 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 10 | 0.19 |
| (2,1936) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 3 | 0.19 |
| (2,1936) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 3 | 0.19 |
| (2,1936) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 3 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 5 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 5 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 5 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 5 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 9 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 9 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 9 | 0.19 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 9 | 0.19 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG2 | 2 | 0.19 |
| (2,1885) | 2:B:145:GLU:HA | 2:B:145:GLU:HG3 | 2 | 0.19 |
| (2,1876) | 2:B:143:ILE:HG21 | 2:B:147:ASN:HB2 | 10 | 0.19 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB2 | 10 | 0.19 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB3 | 10 | 0.19 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 9 | 0.19 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 9 | 0.19 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 9 | 0.19 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 9 | 0.19 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 10 | 0.19 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 10 | 0.19 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 6 | 0.19 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 6 | 0.19 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 7 | 0.19 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 7 | 0.19 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 8 | 0.19 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 8 | 0.19 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 10 | 0.19 |
| (2,1672) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 10 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HD13 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HD12 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HD11 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HD13 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HD12 | 6 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1541) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HD11 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HD13 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HD12 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HD11 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD11 | 1:A:28:ILE:HD11 | 6 | 0.19 |
| (2,1541) | 1:A:51:LEU:HD21 | 1:A:28:ILE:HD11 | 6 | 0.19 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 10 | 0.19 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 10 | 0.19 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 10 | 0.19 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 10 | 0.19 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 4 | 0.19 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 4 | 0.19 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 4 | 0.19 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD2 | 5 | 0.19 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD3 | 5 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 2 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 2 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 4 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 4 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 7 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 7 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 8 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 8 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 10 | 0.19 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 10 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 9 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 9 | 0.19 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 9 | 0.19 |
| (2,1158) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 10 | 0.19 |
| (2,1158) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 10 | 0.19 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 9 | 0.19 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 9 | 0.19 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 1 | 0.19 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 1 | 0.19 |
| (2,1054) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HE2 | 6 | 0.19 |
| (2,1054) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HE3 | 6 | 0.19 |
| (2,1054) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HE2 | 6 | 0.19 |
| (2,1054) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HE3 | 6 | 0.19 |
| (2,1054) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HE2 | 6 | 0.19 |
| (2,1054) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HE3 | 6 | 0.19 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 2 | 0.19 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 2 | 0.19 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 2 | 0.19 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 2 | 0.19 |
| (1,41) | 1:A:45:GLY:N | 1:A:41:PRO:O | 10 | 0.19 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 1 | 0.18 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 1 | 0.18 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 3 | 0.18 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 3 | 0.18 |
| (2,827) | 2:B:108:LEU:HD11 | 2:B:104:VAL:HB | 10 | 0.18 |
| (2,827) | 2:B:108:LEU:HD22 | 2:B:104:VAL:HB | 10 | 0.18 |
| (2,827) | 2:B:108:LEU:HD23 | 2:B:104:VAL:HB | 10 | 0.18 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 10 | 0.18 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 10 | 0.18 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 10 | 0.18 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 10 | 0.18 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 10 | 0.18 |
| (2,677) | 1:A:49:LYS:HB2 | 1:A:49:LYS:HD2 | 6 | 0.18 |
| (2,677) | 1:A:49:LYS:HB3 | 1:A:49:LYS:HD2 | 6 | 0.18 |
| (2,677) | 1:A:49:LYS:HB3 | 1:A:49:LYS:HD3 | 6 | 0.18 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD13 | 3 | 0.18 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD22 | 3 | 0.18 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD21 | 3 | 0.18 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD23 | 3 | 0.18 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 10 | 0.18 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 10 | 0.18 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 10 | 0.18 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 10 | 0.18 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 10 | 0.18 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 10 | 0.18 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 10 | 0.18 |
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 10 | 0.18 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD11 | 9 | 0.18 |
| (2,513) | 1:A:27:LYS:HG2 | 1:A:28:ILE:HD13 | 9 | 0.18 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD11 | 9 | 0.18 |
| (2,513) | 1:A:27:LYS:HG3 | 1:A:28:ILE:HD13 | 9 | 0.18 |
| (2,498) | 1:A:25:GLU:HG2 | 1:A:48:ALA:HB1 | 4 | 0.18 |
| (2,498) | 1:A:25:GLU:HG2 | 1:A:48:ALA:HB3 | 4 | 0.18 |
| (2,498) | 1:A:25:GLU:HG3 | 1:A:48:ALA:HB1 | 4 | 0.18 |
| (2,498) | 1:A:25:GLU:HG3 | 1:A:48:ALA:HB3 | 4 | 0.18 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 2 | 0.18 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 2 | 0.18 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 2 | 0.18 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 2 | 0.18 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 2 | 0.18 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 6 | 0.18 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 4 | 0.18 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 2 | 0.18 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 4 | 0.18 |
| (2,4520) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 6 | 0.18 |
| (2,4512) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 6 | 0.18 |
| (2,4509) | 2:B:142:VAL:HB | 2:B:143:ILE:H | 7 | 0.18 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 2 | 0.18 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 10 | 0.18 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 9 | 0.18 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 5 | 0.18 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 8 | 0.18 |
| (2,4190) | 2:B:132:ILE:HA | 2:B:132:ILE:HG13 | 9 | 0.18 |
| (2,4104) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 6 | 0.18 |
| (2,4098) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 6 | 0.18 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 4 | 0.18 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 3 | 0.18 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 6 | 0.18 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 8 | 0.18 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 9 | 0.18 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 8 | 0.18 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 8 | 0.18 |
| (2,3840) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 6 | 0.18 |
| (2,3840) | 2:B:122:ASP:H | 2:B:122:ASP:HB3 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 7 | 0.18 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 8 | 0.18 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 7 | 0.18 |
| (2,3492) | 2:B:152:GLU:HG2 | 1:A:7:LEU:HB3 | 7 | 0.18 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB2 | 7 | 0.18 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB3 | 7 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 6 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 6 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 6 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 6 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 6 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 6 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 6 | 0.18 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 6 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 6 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 6 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 6 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 6 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 6 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 6 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 10 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 10 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 10 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 10 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 10 | 0.18 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 10 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 10 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 10 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 10 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 10 | 0.18 |
| (2,3392) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 10 | 0.18 |
| (2,3331) | 1:A:14:LEU:HD13 | 2:B:159:ILE:HA | 5 | 0.18 |
| (2,3331) | 1:A:14:LEU:HD22 | 2:B:159:ILE:HA | 5 | 0.18 |
| (2,3331) | 1:A:14:LEU:HD21 | 2:B:159:ILE:HA | 5 | 0.18 |
| (2,3331) | 1:A:14:LEU:HD23 | 2:B:159:ILE:HA | 5 | 0.18 |
| (2,332) | 2:B:165:VAL:H | 2:B:164:SER:HB2 | 2 | 0.18 |
| (2,332) | 2:B:165:VAL:H | 2:B:164:SER:HB3 | 2 | 0.18 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 2 | 0.18 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 2 | 0.18 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 6 | 0.18 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 6 | 0.18 |
| (2,328) | 2:B:163:ALA:H | 2:B:162:LEU:HB2 | 1 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,328) | 2:B:163:ALA:H | 2:B:162:LEU:HB3 | 1 | 0.18 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 3 | 0.18 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 3 | 0.18 |
| (2,3237) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 9 | 0.18 |
| (2,3237) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 9 | 0.18 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 1 | 0.18 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 1 | 0.18 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 1 | 0.18 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB3 | 2 | 0.18 |
| (2,3191) | 2:B:156:ALA:HB3 | 2:B:153:ASP:HB2 | 2 | 0.18 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB2 | 2 | 0.18 |
| (2,3191) | 2:B:156:ALA:HB2 | 2:B:153:ASP:HB3 | 2 | 0.18 |
| (2,3191) | 2:B:156:ALA:HB1 | 2:B:153:ASP:HB2 | 2 | 0.18 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 3 | 0.18 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 3 | 0.18 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 3 | 0.18 |
| (2,3171) | 2:B:154:VAL:HG22 | 2:B:107:TYR:HE1 | 10 | 0.18 |
| (2,3171) | 2:B:154:VAL:HG21 | 2:B:107:TYR:HE1 | 10 | 0.18 |
| (2,3171) | 2:B:154:VAL:HG23 | 2:B:107:TYR:HE1 | 10 | 0.18 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 3 | 0.18 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 3 | 0.18 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 7 | 0.18 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 7 | 0.18 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 3 | 0.18 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 3 | 0.18 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 7 | 0.18 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 7 | 0.18 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 5 | 0.18 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 5 | 0.18 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 5 | 0.18 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 1 | 0.18 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 1 | 0.18 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 10 | 0.18 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 10 | 0.18 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 6 | 0.18 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 6 | 0.18 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 6 | 0.18 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 6 | 0.18 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 10 | 0.18 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 10 | 0.18 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 10 | 0.18 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 2 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 2 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 4 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 4 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 7 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 7 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 8 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 8 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 9 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 9 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 10 | 0.18 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 10 | 0.18 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 5 | 0.18 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 5 | 0.18 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 5 | 0.18 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 8 | 0.18 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 8 | 0.18 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 8 | 0.18 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 1 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 2 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 3 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 3 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 4 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 5 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 6 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 6 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 7 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 8 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 9 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD21 | 2:B:108:LEU:HD23 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD11 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD12 | 2:B:108:LEU:HD13 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD11 | 2:B:108:LEU:HD13 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD23 | 10 | 0.18 |
| (2,2686) | 2:B:108:LEU:HD22 | 2:B:108:LEU:HD21 | 10 | 0.18 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 1 | 0.18 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 1 | 0.18 |
| (2,2627) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 1 | 0.18 |
| (2,2627) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 1 | 0.18 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 8 | 0.18 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 8 | 0.18 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 10 | 0.18 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 10 | 0.18 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 4 | 0.18 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 4 | 0.18 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 4 | 0.18 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 6 | 0.18 |
| (2,2412) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 6 | 0.18 |
| (2,2412) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 6 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 5 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 5 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 7 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 7 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 8 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 8 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 10 | 0.18 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 10 | 0.18 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 7 | 0.18 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 7 | 0.18 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 7 | 0.18 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG22 | 6 | 0.18 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG21 | 6 | 0.18 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG23 | 6 | 0.18 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD21 | 6 | 0.18 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD23 | 6 | 0.18 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG22 | 6 | 0.18 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG21 | 6 | 0.18 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG23 | 6 | 0.18 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 5 | 0.18 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 5 | 0.18 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 5 | 0.18 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 5 | 0.18 |
| (2,2151) | 1:A:15:ILE:HG22 | 1:A:14:LEU:H | 10 | 0.18 |
| (2,2151) | 1:A:15:ILE:HG21 | 1:A:14:LEU:H | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2151) | 1:A:15:ILE:HG23 | 1:A:14:LEU:H | 10 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 2 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 2 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 2 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 3 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 3 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 3 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 5 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 5 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 5 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 7 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 7 | 0.18 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 7 | 0.18 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 3 | 0.18 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 3 | 0.18 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 3 | 0.18 |
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 3 | 0.18 |
| (2,2071) | 1:A:7:LEU:HD22 | 1:A:11:TYR:HE1 | 6 | 0.18 |
| (2,2071) | 1:A:7:LEU:HD21 | 1:A:11:TYR:HE1 | 6 | 0.18 |
| (2,2071) | 1:A:7:LEU:HD23 | 1:A:11:TYR:HE1 | 6 | 0.18 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 4 | 0.18 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 4 | 0.18 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 10 | 0.18 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 10 | 0.18 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 4 | 0.18 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 4 | 0.18 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 10 | 0.18 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 10 | 0.18 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 5 | 0.18 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 5 | 0.18 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 5 | 0.18 |
| (2,1989) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 5 | 0.18 |
| (2,1989) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 5 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 4 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 4 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 6 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 6 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 7 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 7 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 8 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 8 | 0.18 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 9 | 0.18 |
| (2,1967) | 2:B:157:GLN:HA | 2:B:157:GLN:HG2 | 7 | 0.18 |
| (2,1967) | 2:B:157:GLN:HA | 2:B:157:GLN:HG3 | 7 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD12 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD11 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:146:LEU:HD13 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD12 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD11 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD11 | 2:B:108:LEU:HD13 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD12 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD11 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD13 | 2:B:108:LEU:HD13 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD12 | 6 | 0.18 |
| (2,1919) | 2:B:151:ILE:HD12 | 2:B:108:LEU:HD13 | 6 | 0.18 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 7 | 0.18 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 7 | 0.18 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 7 | 0.18 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 7 | 0.18 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 8 | 0.18 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 8 | 0.18 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 8 | 0.18 |
| (2,1893) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 8 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG12 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG11 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG13 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG12 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG11 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG13 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG12 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG11 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG13 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG22 | 10 | 0.18 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG23 | 10 | 0.18 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 3 | 0.18 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 3 | 0.18 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB2 | 5 | 0.18 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB3 | 5 | 0.18 |
| (2,1809) | 2:B:132:ILE:HG22 | 1:A:18:ASP:HB2 | 7 | 0.18 |
| (2,1809) | 2:B:132:ILE:HG23 | 1:A:18:ASP:HB2 | 7 | 0.18 |
| (2,1721) | 2:B:122:ASP:HA | 2:B:125:LYS:HG2 | 10 | 0.18 |
| (2,1721) | 2:B:122:ASP:HA | 2:B:125:LYS:HG3 | 10 | 0.18 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 8 | 0.18 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 8 | 0.18 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 8 | 0.18 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 8 | 0.18 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 5 | 0.18 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 5 | 0.18 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 5 | 0.18 |
| (2,1391) | 1:A:24:THR:HG21 | 1:A:27:LYS:HE3 | 8 | 0.18 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE2 | 8 | 0.18 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE3 | 8 | 0.18 |
| (2,1391) | 1:A:24:THR:HG23 | 1:A:27:LYS:HE3 | 8 | 0.18 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 7 | 0.18 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 7 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 1 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 1 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 2 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 2 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 3 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 3 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 4 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 4 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 5 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 5 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 6 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 6 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 7 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 7 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 8 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 8 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 9 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 9 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.18 |
| (2,1325) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.18 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 5 | 0.18 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 5 | 0.18 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 5 | 0.18 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 7 | 0.18 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 7 | 0.18 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 7 | 0.18 |
| (2,1219) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 6 | 0.18 |
| (2,1219) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 6 | 0.18 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 1 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 1 | 0.18 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 3 | 0.18 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 3 | 0.18 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 6 | 0.18 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 6 | 0.18 |
| (2,1175) | 2:B:154:VAL:HG12 | 2:B:154:VAL:HA | 9 | 0.18 |
| (2,1175) | 2:B:154:VAL:HG13 | 2:B:154:VAL:HA | 9 | 0.18 |
| (2,1175) | 2:B:154:VAL:HG22 | 2:B:154:VAL:HA | 9 | 0.18 |
| (2,1175) | 2:B:154:VAL:HG21 | 2:B:154:VAL:HA | 9 | 0.18 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 1 | 0.18 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 1 | 0.18 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 2 | 0.18 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 2 | 0.18 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 2 | 0.18 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG2 | 10 | 0.18 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG3 | 10 | 0.18 |
| (1,82) | 2:B:129:SER:H | 2:B:125:LYS:O | 10 | 0.18 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 4 | 0.18 |
| (2,761) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 1 | 0.17 |
| (2,761) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 1 | 0.17 |
| (2,761) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 1 | 0.17 |
| (2,695) | 1:A:51:LEU:HD12 | 1:A:48:ALA:HA | 1 | 0.17 |
| (2,695) | 1:A:51:LEU:HD11 | 1:A:48:ALA:HA | 1 | 0.17 |
| (2,695) | 1:A:51:LEU:HD13 | 1:A:48:ALA:HA | 1 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 1 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 1 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 3 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 3 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 4 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 4 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 8 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 8 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 10 | 0.17 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 10 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 2 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 2 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 2 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 2 | 0.17 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 2 | 0.17 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 2 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 2 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 2 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 2 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 7 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 9 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 9 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 9 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 9 | 0.17 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 9 | 0.17 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 9 | 0.17 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 9 | 0.17 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 9 | 0.17 |
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 9 | 0.17 |
| (2,587) | 1:A:37:VAL:HG12 | 2:B:112:LEU:HD23 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD22 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD21 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD21 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 8 | 0.17 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG22 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG21 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG23 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HD12 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG22 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG21 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG23 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG22 | 8 | 0.17 |
| (2,567) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG21 | 8 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 7 | 0.17 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 7 | 0.17 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 7 | 0.17 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 7 | 0.17 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 7 | 0.17 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 6 | 0.17 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 5 | 0.17 |
| (2,4556) | 2:B:161:LYS:HA | 2:B:161:LYS:H | 5 | 0.17 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 1 | 0.17 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 2 | 0.17 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 5 | 0.17 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 10 | 0.17 |
| (2,4517) | 2:B:144:SER:HA | 2:B:143:ILE:HB | 4 | 0.17 |
| (2,4517) | 2:B:144:SER:HA | 2:B:143:ILE:HB | 10 | 0.17 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 2 | 0.17 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 6 | 0.17 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 7 | 0.17 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 8 | 0.17 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 10 | 0.17 |
| (2,4455) | 2:B:124:LYS:HA | 2:B:127:LEU:HB3 | 7 | 0.17 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 1 | 0.17 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 2 | 0.17 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 5 | 0.17 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 7 | 0.17 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 10 | 0.17 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD12 | 2 | 0.17 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD11 | 2 | 0.17 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD13 | 2 | 0.17 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD21 | 2 | 0.17 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 4 | 0.17 |
| (2,4251) | 1:A:15:ILE:HA | 2:B:103:TYR:HA | 2 | 0.17 |
| (2,4208) | 2:B:165:VAL:HA | 2:B:165:VAL:HB | 9 | 0.17 |
| (2,4182) | 2:B:124:LYS:HA | 2:B:127:LEU:HB3 | 7 | 0.17 |
| (2,4119) | 2:B:155:ILE:HB | 2:B:152:GLU:HA | 5 | 0.17 |
| (2,4093) | 2:B:132:ILE:HB | 2:B:127:LEU:HB2 | 5 | 0.17 |
| (2,4083) | 2:B:124:LYS:HA | 2:B:127:LEU:HB3 | 7 | 0.17 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 1 | 0.17 |
| (2,4014) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 2 | 0.17 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 4 | 0.17 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 4 | 0.17 |
| (2,3999) | 2:B:160:GLY:H | 2:B:162:LEU:H | 6 | 0.17 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,3814) | 2:B:116:SER:H | 2:B:117:SER:H | 3 | 0.17 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 4 | 0.17 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 7 | 0.17 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 2 | 0.17 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 5 | 0.17 |
| (2,3528) | 1:A:5:SER:H | 1:A:3:SER:HA | 9 | 0.17 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 3 | 0.17 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 4 | 0.17 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 6 | 0.17 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 10 | 0.17 |
| (2,3492) | 2:B:152:GLU:HG2 | 1:A:7:LEU:HB3 | 9 | 0.17 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB2 | 9 | 0.17 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB3 | 9 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 5 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 5 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 5 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 5 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 5 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 5 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 5 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 5 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 7 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 7 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 7 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 7 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 7 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 7 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 7 | 0.17 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 7 | 0.17 |
| (2,3416) | 2:B:101:MET:HE2 | 1:A:17:HIS:HD2 | 4 | 0.17 |
| (2,3416) | 2:B:101:MET:HE1 | 1:A:17:HIS:HD2 | 4 | 0.17 |
| (2,3416) | 2:B:101:MET:HE3 | 1:A:17:HIS:HD2 | 4 | 0.17 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB2 | 5 | 0.17 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB3 | 5 | 0.17 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB2 | 5 | 0.17 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB3 | 5 | 0.17 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB2 | 10 | 0.17 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB3 | 10 | 0.17 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB2 | 10 | 0.17 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB3 | 10 | 0.17 |
| (2,3392) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 5 | 0.17 |
| (2,3392) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 5 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3392) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 5 | 0.17 |
| (2,3392) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 5 | 0.17 |
| (2,3392) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 5 | 0.17 |
| (2,3389) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 10 | 0.17 |
| (2,3389) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 10 | 0.17 |
| (2,3389) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 10 | 0.17 |
| (2,3389) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 10 | 0.17 |
| (2,3389) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD12 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD11 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD13 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD12 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD11 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD13 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:109:LEU:HD13 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD12 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD11 | 10 | 0.17 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD13 | 10 | 0.17 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 1 | 0.17 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 1 | 0.17 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 1 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 2 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 2 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 2 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 2 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 2 | 0.17 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 2 | 0.17 |
| (2,3300) | 1:A:2:ALA:HB2 | 2:B:152:GLU:HG3 | 6 | 0.17 |
| (2,3300) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HG3 | 6 | 0.17 |
| (2,3300) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HG3 | 6 | 0.17 |
| (2,328) | 2:B:163:ALA:H | 2:B:162:LEU:HB2 | 8 | 0.17 |
| (2,328) | 2:B:163:ALA:H | 2:B:162:LEU:HB3 | 8 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 5 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 5 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 5 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 5 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 5 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 8 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 8 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 8 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 8 | 0.17 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 8 | 0.17 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 6 | 0.17 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 6 | 0.17 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 9 | 0.17 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 9 | 0.17 |
| (2,3140) | 2:B:151:ILE:HD11 | 2:B:149:LYS:H | 6 | 0.17 |
| (2,3140) | 2:B:151:ILE:HD13 | 2:B:149:LYS:H | 6 | 0.17 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG2 | 2 | 0.17 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG3 | 2 | 0.17 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 6 | 0.17 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 6 | 0.17 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 6 | 0.17 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 6 | 0.17 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 6 | 0.17 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 6 | 0.17 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 6 | 0.17 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 7 | 0.17 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 7 | 0.17 |
| (2,3056) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 7 | 0.17 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 1 | 0.17 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 1 | 0.17 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 1 | 0.17 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 1 | 0.17 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD12 | 2 | 0.17 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD11 | 2 | 0.17 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD13 | 2 | 0.17 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD12 | 8 | 0.17 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD11 | 8 | 0.17 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD13 | 8 | 0.17 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE1 | 8 | 0.17 |
| (2,3021) | 2:B:139:LEU:HD22 | 2:B:103:TYR:HE2 | 8 | 0.17 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE1 | 8 | 0.17 |
| (2,3021) | 2:B:139:LEU:HD21 | 2:B:103:TYR:HE2 | 8 | 0.17 |
| (2,3021) | 2:B:139:LEU:HD23 | 2:B:103:TYR:HE2 | 8 | 0.17 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB1 | 2 | 0.17 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB3 | 2 | 0.17 |
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2979) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 4 | 0.17 |
| (2,2979) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 4 | 0.17 |
| (2,2979) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 4 | 0.17 |
| (2,2976) | 2:B:134:ALA:HB2 | 2:B:135:ASP:HB3 | 8 | 0.17 |
| (2,2976) | 2:B:134:ALA:HB1 | 2:B:135:ASP:HB3 | 8 | 0.17 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB2 | 8 | 0.17 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB3 | 8 | 0.17 |
| (2,2871) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 1 | 0.17 |
| (2,2871) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 1 | 0.17 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 8 | 0.17 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 8 | 0.17 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 8 | 0.17 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 1 | 0.17 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 1 | 0.17 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 1 | 0.17 |
| (2,282) | 2:B:140:ASN:H | 2:B:141:LYS:HB2 | 6 | 0.17 |
| (2,282) | 2:B:140:ASN:H | 2:B:141:LYS:HB3 | 6 | 0.17 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 5 | 0.17 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 5 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 2 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 2 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 2 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 2 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 3 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 3 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 3 | 0.17 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 3 | 0.17 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 1 | 0.17 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 1 | 0.17 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 3 | 0.17 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 3 | 0.17 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 5 | 0.17 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 5 | 0.17 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 6 | 0.17 |
| (2,2737) | 2:B:112:LEU:HB2 | 2:B:112:LEU:HB3 | 6 | 0.17 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 7 | 0.17 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 7 | 0.17 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 7 | 0.17 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 7 | 0.17 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 9 | 0.17 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 9 | 0.17 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 9 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 9 | 0.17 |
| (2,2717) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HD21 | 1 | 0.17 |
| (2,2717) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HD21 | 1 | 0.17 |
| (2,2717) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HD21 | 1 | 0.17 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 5 | 0.17 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 5 | 0.17 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD21 | 5 | 0.17 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD22 | 5 | 0.17 |
| (2,2579) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HD21 | 5 | 0.17 |
| (2,2538) | 1:A:58:SER:HB2 | 1:A:55:ASN:HB2 | 6 | 0.17 |
| (2,2538) | 1:A:58:SER:HB2 | 1:A:55:ASN:HB3 | 6 | 0.17 |
| (2,2538) | 1:A:58:SER:HB3 | 1:A:55:ASN:HB3 | 6 | 0.17 |
| (2,2493) | 1:A:51:LEU:H | 1:A:51:LEU:HD12 | 6 | 0.17 |
| (2,2493) | 1:A:51:LEU:H | 1:A:51:LEU:HD11 | 6 | 0.17 |
| (2,2493) | 1:A:51:LEU:H | 1:A:51:LEU:HD13 | 6 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 2 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 2 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 2 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 2 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 2 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 2 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 5 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 5 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 5 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 5 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 5 | 0.17 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 5 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG22 | 8 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB3 | 2:B:126:ILE:HG21 | 8 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG22 | 8 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG21 | 8 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB2 | 2:B:126:ILE:HG23 | 8 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HD12 | 8 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG22 | 8 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG21 | 8 | 0.17 |
| (2,2346) | 1:A:34:ALA:HB1 | 2:B:126:ILE:HG23 | 8 | 0.17 |
| (2,2282) | 1:A:27:LYS:HG2 | 1:A:27:LYS:H | 9 | 0.17 |
| (2,2282) | 1:A:27:LYS:HG3 | 1:A:27:LYS:H | 9 | 0.17 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 1 | 0.17 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 1 | 0.17 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 1 | 0.17 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 6 | 0.17 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 6 | 0.17 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 6 | 0.17 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 9 | 0.17 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 9 | 0.17 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 9 | 0.17 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 9 | 0.17 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 4 | 0.17 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 4 | 0.17 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 4 | 0.17 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 6 | 0.17 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 6 | 0.17 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 6 | 0.17 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 1 | 0.17 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 1 | 0.17 |
| (2,2034) | 1:A:2:ALA:HB2 | 1:A:6:GLU:H | 3 | 0.17 |
| (2,2034) | 1:A:2:ALA:HB3 | 1:A:6:GLU:H | 3 | 0.17 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 2 | 0.17 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 2 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 1 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 1 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 2 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 2 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 7 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 7 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 8 | 0.17 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 8 | 0.17 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 4 | 0.17 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 4 | 0.17 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 6 | 0.17 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 6 | 0.17 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 9 | 0.17 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 9 | 0.17 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 5 | 0.17 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 5 | 0.17 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD12 | 7 | 0.17 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD13 | 7 | 0.17 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD22 | 7 | 0.17 |
| (2,1848) | 2:B:139:LEU:HA | 2:B:139:LEU:HD23 | 7 | 0.17 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 5 | 0.17 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 5 | 0.17 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 5 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 5 | 0.17 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 5 | 0.17 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 7 | 0.17 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 7 | 0.17 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 7 | 0.17 |
| (2,1393) | 1:A:24:THR:HG21 | 1:A:26:ASP:HB3 | 10 | 0.17 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB2 | 10 | 0.17 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB3 | 10 | 0.17 |
| (2,1393) | 1:A:24:THR:HG23 | 1:A:26:ASP:HB3 | 10 | 0.17 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 3 | 0.17 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 3 | 0.17 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 4 | 0.17 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 4 | 0.17 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 5 | 0.17 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 5 | 0.17 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 6 | 0.17 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 6 | 0.17 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 6 | 0.17 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 6 | 0.17 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 9 | 0.17 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 9 | 0.17 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 9 | 0.17 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD2 | 1 | 0.17 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD3 | 1 | 0.17 |
| (2,1219) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 5 | 0.17 |
| (2,1219) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 5 | 0.17 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD13 | 5 | 0.17 |
| (2,1206) | 2:B:159:ILE:HB | 2:B:159:ILE:HD12 | 5 | 0.17 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 10 | 0.17 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 10 | 0.17 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 1 | 0.17 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 1 | 0.17 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 1 | 0.17 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 4 | 0.17 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 4 | 0.17 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 4 | 0.17 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG22 | 1 | 0.17 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG21 | 1 | 0.17 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG22 | 3 | 0.17 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG21 | 3 | 0.17 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG22 | 4 | 0.17 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG21 | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 7 | 0.17 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 7 | 0.17 |
| (2,1083) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 7 | 0.17 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 5 | 0.17 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 5 | 0.17 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 8 | 0.17 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 8 | 0.17 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG2 | 1 | 0.17 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG3 | 1 | 0.17 |
| (2,1034) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 9 | 0.17 |
| (2,1034) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 9 | 0.17 |
| (2,1034) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 9 | 0.17 |
| (2,1034) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 9 | 0.17 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 2 | 0.17 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 3 | 0.17 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 5 | 0.17 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 6 | 0.17 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 7 | 0.17 |
| (1,81) | 2:B:129:SER:N | 2:B:125:LYS:O | 1 | 0.17 |
| (1,75) | 2:B:126:ILE:N | 2:B:122:ASP:O | 4 | 0.17 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 9 | 0.16 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 9 | 0.16 |
| (2,850) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 9 | 0.16 |
| (2,850) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 9 | 0.16 |
| (2,833) | 2:B:109:LEU:HB2 | 2:B:110:ALA:HA | 4 | 0.16 |
| (2,833) | 2:B:109:LEU:HB3 | 2:B:110:ALA:HA | 4 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 1 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 1 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 1 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 2 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 2 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 2 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 3 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 3 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 3 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 4 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 4 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 4 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 5 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 5 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 5 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 7 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 7 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 8 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 8 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 8 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 9 | 0.16 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 9 | 0.16 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 9 | 0.16 |
| (2,677) | 1:A:49:LYS:HB2 | 1:A:49:LYS:HD2 | 7 | 0.16 |
| (2,677) | 1:A:49:LYS:HB3 | 1:A:49:LYS:HD2 | 7 | 0.16 |
| (2,677) | 1:A:49:LYS:HB3 | 1:A:49:LYS:HD3 | 7 | 0.16 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG12 | 1 | 0.16 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG11 | 1 | 0.16 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG13 | 1 | 0.16 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG21 | 1 | 0.16 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA2 | 5 | 0.16 |
| (2,595) | 1:A:37:VAL:HG12 | 2:B:114:GLY:HA3 | 5 | 0.16 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA2 | 5 | 0.16 |
| (2,595) | 1:A:37:VAL:HG11 | 2:B:114:GLY:HA3 | 5 | 0.16 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA2 | 5 | 0.16 |
| (2,595) | 1:A:37:VAL:HG13 | 2:B:114:GLY:HA3 | 5 | 0.16 |
| (2,595) | 1:A:37:VAL:HG11 | 1:A:39:VAL:HA | 5 | 0.16 |
| (2,595) | 1:A:37:VAL:HG12 | 1:A:39:VAL:HA | 5 | 0.16 |
| (2,595) | 1:A:37:VAL:HG13 | 1:A:39:VAL:HA | 5 | 0.16 |
| (2,587) | 1:A:37:VAL:HG12 | 2:B:112:LEU:HD23 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD22 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD21 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD21 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 2 | 0.16 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 2 | 0.16 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 1 | 0.16 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 9 | 0.16 |
| (2,4524) | 2:B:146:LEU:H | 2:B:146:LEU:HG | 3 | 0.16 |
| (2,4517) | 2:B:144:SER:HA | 2:B:143:ILE:HB | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,4509) | 2:B:142:VAL:HB | 2:B:143:ILE:H | 8 | 0.16 |
| (2,4422) | 2:B:108:LEU:HA | 2:B:107:TYR:H | 5 | 0.16 |
| (2,4342) | 1:A:41:PRO:HA | 1:A:40:GLU:H | 7 | 0.16 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 2 | 0.16 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 3 | 0.16 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD12 | 10 | 0.16 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD11 | 10 | 0.16 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD13 | 10 | 0.16 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD21 | 10 | 0.16 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 5 | 0.16 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 6 | 0.16 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 8 | 0.16 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 9 | 0.16 |
| (2,4084) | 2:B:124:LYS:HA | 2:B:124:LYS:HD2 | 6 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 1 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 2 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 3 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 4 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 5 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 6 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 7 | 0.16 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 10 | 0.16 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 10 | 0.16 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 2 | 0.16 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 2 | 0.16 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 6 | 0.16 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 6 | 0.16 |
| (2,3999) | 2:B:160:GLY:H | 2:B:162:LEU:H | 4 | 0.16 |
| (2,3954) | 2:B:143:ILE:H | 2:B:107:TYR:HE2 | 6 | 0.16 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 10 | 0.16 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 9 | 0.16 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 2 | 0.16 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 5 | 0.16 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 10 | 0.16 |
| (2,3804) | 2:B:115:ASN:H | 2:B:116:SER:HA | 8 | 0.16 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 1 | 0.16 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 7 | 0.16 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 4 | 0.16 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 9 | 0.16 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 2 | 0.16 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 5 | 0.16 |
| (2,3416) | 2:B:101:MET:HE2 | 1:A:17:HIS:HD2 | 6 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,3416) | 2:B:101:MET:HE1 | 1:A:17:HIS:HD2 | 6 | 0.16 |
| (2,3416) | 2:B:101:MET:HE3 | 1:A:17:HIS:HD2 | 6 | 0.16 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB2 | 9 | 0.16 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB3 | 9 | 0.16 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB2 | 9 | 0.16 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB3 | 9 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD12 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD11 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD13 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG21 | 2:B:109:LEU:HD13 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD12 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD11 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD13 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD12 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD11 | 8 | 0.16 |
| (2,3393) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD13 | 8 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 5 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 5 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 5 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 5 | 0.16 |
| (2,3389) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 5 | 0.16 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 7 | 0.16 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 7 | 0.16 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 7 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG22 | 2:B:101:MET:HE2 | 1 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE2 | 1 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE3 | 1 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE2 | 1 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE1 | 1 | 0.16 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE3 | 1 | 0.16 |
| (2,3237) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 6 | 0.16 |
| (2,3237) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 6 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 4 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 4 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 4 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 7 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 7 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 8 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 8 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 8 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 9 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 9 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 9 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 10 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 10 | 0.16 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 10 | 0.16 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 4 | 0.16 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 4 | 0.16 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 4 | 0.16 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 4 | 0.16 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 7 | 0.16 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 7 | 0.16 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 7 | 0.16 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 7 | 0.16 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 7 | 0.16 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 2 | 0.16 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 2 | 0.16 |
| (2,3166) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG22 | 2 | 0.16 |
| (2,3166) | 2:B:149:LYS:HB3 | 2:B:154:VAL:HG22 | 2 | 0.16 |
| (2,3166) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG21 | 2 | 0.16 |
| (2,3166) | 2:B:149:LYS:HB3 | 2:B:154:VAL:HG21 | 2 | 0.16 |
| (2,3166) | 2:B:149:LYS:HB2 | 2:B:154:VAL:HG23 | 2 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 1 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 1 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 2 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 2 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 4 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 4 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 5 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 5 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 8 | 0.16 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 8 | 0.16 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG22 | 9 | 0.16 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG21 | 9 | 0.16 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG21 | 9 | 0.16 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG23 | 9 | 0.16 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 10 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 10 | 0.16 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 10 | 0.16 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 10 | 0.16 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 10 | 0.16 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 10 | 0.16 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 10 | 0.16 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 3 | 0.16 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 3 | 0.16 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 5 | 0.16 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 5 | 0.16 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG21 | 1 | 0.16 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG23 | 1 | 0.16 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 4 | 0.16 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 4 | 0.16 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 4 | 0.16 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 4 | 0.16 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 2 | 0.16 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 2 | 0.16 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 2 | 0.16 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD12 | 6 | 0.16 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD11 | 6 | 0.16 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD13 | 6 | 0.16 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD12 | 9 | 0.16 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD11 | 9 | 0.16 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD13 | 9 | 0.16 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 8 | 0.16 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 8 | 0.16 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 8 | 0.16 |
| (2,3010) | 2:B:138:ARG:HG2 | 2:B:135:ASP:H | 7 | 0.16 |
| (2,3010) | 2:B:138:ARG:HG3 | 2:B:135:ASP:H | 7 | 0.16 |
| (2,2976) | 2:B:134:ALA:HB2 | 2:B:135:ASP:HB3 | 7 | 0.16 |
| (2,2976) | 2:B:134:ALA:HB1 | 2:B:135:ASP:HB3 | 7 | 0.16 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB2 | 7 | 0.16 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB3 | 7 | 0.16 |
| (2,296) | 2:B:144:SER:H | 2:B:141:LYS:HG2 | 9 | 0.16 |
| (2,296) | 2:B:144:SER:H | 2:B:141:LYS:HG3 | 9 | 0.16 |
| (2,2871) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 2 | 0.16 |
| (2,2871) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 2 | 0.16 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 10 | 0.16 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 10 | 0.16 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 10 | 0.16 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 3 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 3 | 0.16 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 8 | 0.16 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 8 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 1 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 1 | 0.16 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 1 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 2 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 2 | 0.16 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 2 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 3 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 3 | 0.16 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 3 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 4 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 4 | 0.16 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 4 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 7 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 7 | 0.16 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 7 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 8 | 0.16 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 8 | 0.16 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 8 | 0.16 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 5 | 0.16 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 5 | 0.16 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 5 | 0.16 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 5 | 0.16 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 5 | 0.16 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 5 | 0.16 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 5 | 0.16 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 9 | 0.16 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 9 | 0.16 |
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 9 | 0.16 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 10 | 0.16 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 10 | 0.16 |
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 10 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 1 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 1 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 3 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 3 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 4 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 4 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 10 | 0.16 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 10 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 1 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 1 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 2 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 2 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 3 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 3 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 4 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 4 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 5 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 5 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 6 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 6 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 7 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 7 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 8 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 8 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 9 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 9 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 10 | 0.16 |
| (2,2679) | 2:B:108:LEU:HB2 | 2:B:108:LEU:HB3 | 10 | 0.16 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 4 | 0.16 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 4 | 0.16 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 6 | 0.16 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 6 | 0.16 |
| (2,2538) | 1:A:58:SER:HB2 | 1:A:55:ASN:HB2 | 2 | 0.16 |
| (2,2538) | 1:A:58:SER:HB2 | 1:A:55:ASN:HB3 | 2 | 0.16 |
| (2,2538) | 1:A:58:SER:HB3 | 1:A:55:ASN:HB3 | 2 | 0.16 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 4 | 0.16 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 4 | 0.16 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 9 | 0.16 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 9 | 0.16 |
| (2,2328) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 9 | 0.16 |
| (2,2256) | 1:A:25:GLU:HG3 | 1:A:29:ASN:HD22 | 1 | 0.16 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD21 | 1 | 0.16 |
| (2,2256) | 1:A:25:GLU:HG2 | 1:A:29:ASN:HD22 | 1 | 0.16 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 2 | 0.16 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 2 | 0.16 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 2 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG22 | 4 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG21 | 4 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG23 | 4 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD21 | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD23 | 4 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG22 | 4 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG21 | 4 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG23 | 4 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG22 | 10 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG21 | 10 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG23 | 10 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD21 | 10 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD23 | 10 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG22 | 10 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG21 | 10 | 0.16 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG23 | 10 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD23 | 1:A:27:LYS:HE3 | 2 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD12 | 1:A:27:LYS:HE2 | 2 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD12 | 1:A:27:LYS:HE3 | 2 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD11 | 1:A:27:LYS:HE2 | 2 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD11 | 1:A:27:LYS:HE3 | 2 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD22 | 1:A:27:LYS:HE2 | 2 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD22 | 1:A:27:LYS:HE3 | 2 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD21 | 1:A:27:LYS:HE3 | 2 | 0.16 |
| (2,2166) | 1:A:16:LEU:HD23 | 1:A:27:LYS:HE2 | 2 | 0.16 |
| (2,2160) | 1:A:16:LEU:HD12 | 1:A:21:VAL:H | 4 | 0.16 |
| (2,2160) | 1:A:16:LEU:HD11 | 1:A:21:VAL:H | 4 | 0.16 |
| (2,2160) | 1:A:16:LEU:HD13 | 1:A:21:VAL:H | 4 | 0.16 |
| (2,2160) | 1:A:16:LEU:HD23 | 1:A:21:VAL:H | 4 | 0.16 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 1 | 0.16 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 1 | 0.16 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 1 | 0.16 |
| (2,206) | 2:B:115:ASN:H | 2:B:111:ALA:H | 6 | 0.16 |
| (2,206) | 2:B:115:ASN:H | 2:B:112:LEU:H | 6 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 2 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 2 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 2 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 3 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 3 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 3 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 4 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 4 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 4 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 5 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 5 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 5 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 6 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 6 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 6 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 9 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 9 | 0.16 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 9 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 3 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 3 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 5 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 5 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 6 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 6 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB2 | 9 | 0.16 |
| (2,2014) | 2:B:166:PRO:HA | 2:B:166:PRO:HB3 | 9 | 0.16 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 3 | 0.16 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 3 | 0.16 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 7 | 0.16 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 7 | 0.16 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 8 | 0.16 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 8 | 0.16 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 10 | 0.16 |
| (2,2005) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 10 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 1 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 1 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 1 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 2 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 2 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 2 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 3 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 3 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 3 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 4 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 4 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 4 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 5 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 5 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 5 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 6 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 6 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 6 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 7 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 7 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 8 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 8 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 8 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 9 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 9 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 9 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD3 | 10 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HD3 | 10 | 0.16 |
| (2,1992) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HD2 | 10 | 0.16 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD12 | 3 | 0.16 |
| (2,1974) | 2:B:159:ILE:HA | 2:B:159:ILE:HD13 | 3 | 0.16 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 1 | 0.16 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 1 | 0.16 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 7 | 0.16 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 7 | 0.16 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 8 | 0.16 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 8 | 0.16 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG3 | 6 | 0.16 |
| (2,1719) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HG2 | 6 | 0.16 |
| (2,1719) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HG2 | 6 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 1 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 1 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 1 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 1 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 1 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 6 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 6 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 6 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 6 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 6 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 10 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 10 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 10 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 10 | 0.16 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 10 | 0.16 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG2 | 6 | 0.16 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG3 | 6 | 0.16 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG2 | 6 | 0.16 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG3 | 6 | 0.16 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 9 | 0.16 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 9 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 9 | 0.16 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 10 | 0.16 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 10 | 0.16 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 3 | 0.16 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 3 | 0.16 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 3 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD22 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD21 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD23 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD22 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD21 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD23 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD22 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD21 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD23 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD22 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD21 | 1 | 0.16 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD23 | 1 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 2 | 0.16 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 2 | 0.16 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 5 | 0.16 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 5 | 0.16 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 8 | 0.16 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 8 | 0.16 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD11 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD13 | 8 | 0.16 |
| (2,1132) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 8 | 0.16 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD21 | 8 | 0.16 |
| (2,1132) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 8 | 0.16 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD12 | 8 | 0.16 |
| (2,1132) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 8 | 0.16 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 10 | 0.16 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 10 | 0.16 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 8 | 0.16 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 8 | 0.16 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 8 | 0.16 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 10 | 0.16 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 10 | 0.16 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 10 | 0.16 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG22 | 10 | 0.16 |
| (2,1110) | 2:B:143:ILE:HA | 2:B:143:ILE:HG21 | 10 | 0.16 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG2 | 5 | 0.16 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG3 | 5 | 0.16 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 10 | 0.16 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 10 | 0.16 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 10 | 0.16 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 1 | 0.16 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 4 | 0.16 |
| (1,84) | 2:B:139:LEU:H | 2:B:135:ASP:O | 8 | 0.16 |
| (1,81) | 2:B:129:SER:N | 2:B:125:LYS:O | 10 | 0.16 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 1 | 0.16 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 6 | 0.16 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 8 | 0.16 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 1 | 0.16 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 3 | 0.16 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 2 | 0.16 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 5 | 0.16 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 6 | 0.16 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 7 | 0.16 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 8 | 0.16 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 9 | 0.16 |
| (1,19) | 1:A:16:LEU:N | 1:A:12:SER:O | 1 | 0.16 |
| (1,13) | 1:A:13:ALA:N | 1:A:9:CYS:O | 6 | 0.16 |
| (2,920) | 2:B:122:ASP:HA | 2:B:125:LYS:HG2 | 10 | 0.15 |
| (2,920) | 2:B:122:ASP:HA | 2:B:125:LYS:HG3 | 10 | 0.15 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 5 | 0.15 |
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,850) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 4 | 0.15 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 4 | 0.15 |
| (2,850) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 4 | 0.15 |
| (2,850) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 4 | 0.15 |
| (2,829) | 2:B:108:LEU:HD12 | 2:B:154:VAL:HB | 10 | 0.15 |
| (2,829) | 2:B:108:LEU:HD13 | 2:B:154:VAL:HB | 10 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 3 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 3 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 3 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 3 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 3 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 9 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 9 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 9 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 9 | 0.15 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 9 | 0.15 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB2 | 10 | 0.15 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB3 | 10 | 0.15 |
| (2,695) | 1:A:51:LEU:HD12 | 1:A:48:ALA:HA | 2 | 0.15 |
| (2,695) | 1:A:51:LEU:HD11 | 1:A:48:ALA:HA | 2 | 0.15 |
| (2,695) | 1:A:51:LEU:HD13 | 1:A:48:ALA:HA | 2 | 0.15 |
| (2,695) | 1:A:51:LEU:HD12 | 1:A:48:ALA:HA | 10 | 0.15 |
| (2,695) | 1:A:51:LEU:HD11 | 1:A:48:ALA:HA | 10 | 0.15 |
| (2,695) | 1:A:51:LEU:HD13 | 1:A:48:ALA:HA | 10 | 0.15 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 6 | 0.15 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 6 | 0.15 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 6 | 0.15 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 10 | 0.15 |
| (2,679) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 10 | 0.15 |
| (2,679) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 10 | 0.15 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 5 | 0.15 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 5 | 0.15 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB2 | 9 | 0.15 |
| (2,672) | 1:A:49:LYS:HA | 1:A:49:LYS:HB3 | 9 | 0.15 |
| (2,671) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 7 | 0.15 |
| (2,671) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 7 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD13 | 5 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD22 | 5 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD21 | 5 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD23 | 5 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD13 | 10 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD22 | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD21 | 10 | 0.15 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD23 | 10 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG12 | 7 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG11 | 7 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG13 | 7 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG21 | 7 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG12 | 8 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG11 | 8 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG13 | 8 | 0.15 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG21 | 8 | 0.15 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 5 | 0.15 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 5 | 0.15 |
| (2,555) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HE2 | 9 | 0.15 |
| (2,555) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HE3 | 9 | 0.15 |
| (2,555) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HE2 | 9 | 0.15 |
| (2,555) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HE3 | 9 | 0.15 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 7 | 0.15 |
| (2,4557) | 2:B:161:LYS:HD2 | 2:B:161:LYS:H | 9 | 0.15 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 10 | 0.15 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 6 | 0.15 |
| (2,4524) | 2:B:146:LEU:H | 2:B:146:LEU:HG | 4 | 0.15 |
| (2,4520) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 5 | 0.15 |
| (2,4512) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 2 | 0.15 |
| (2,4509) | 2:B:142:VAL:HB | 2:B:143:ILE:H | 6 | 0.15 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 1 | 0.15 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 3 | 0.15 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 4 | 0.15 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 5 | 0.15 |
| (2,4490) | 2:B:137:ASP:H | 2:B:137:ASP:HA | 9 | 0.15 |
| (2,4446) | 2:B:120:ALA:HA | 2:B:140:ASN:HA | 1 | 0.15 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 9 | 0.15 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 2 | 0.15 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 6 | 0.15 |
| (2,4251) | 1:A:15:ILE:HA | 2:B:103:TYR:HA | 1 | 0.15 |
| (2,4251) | 1:A:15:ILE:HA | 2:B:103:TYR:HA | 10 | 0.15 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 1 | 0.15 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 2 | 0.15 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 5 | 0.15 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 7 | 0.15 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 10 | 0.15 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 2 | 0.15 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 7 | 0.15 |
| (2,4204) | 2:B:155:ILE:HD12 | 2:B:155:ILE:HB | 9 | 0.15 |
| (2,4191) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 6 | 0.15 |
| (2,4136) | 1:A:22:THR:HA | 1:A:22:THR:HB | 6 | 0.15 |
| (2,4119) | 2:B:155:ILE:HB | 2:B:152:GLU:HA | 4 | 0.15 |
| (2,4104) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 2 | 0.15 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 8 | 0.15 |
| (2,4035) | 1:A:39:VAL:HA | 1:A:39:VAL:HB | 9 | 0.15 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 2 | 0.15 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 3 | 0.15 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 1 | 0.15 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 1 | 0.15 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 2 | 0.15 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 5 | 0.15 |
| (2,3842) | 2:B:122:ASP:H | 2:B:119:SER:HA | 6 | 0.15 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 6 | 0.15 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 7 | 0.15 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB2 | 1 | 0.15 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB3 | 1 | 0.15 |
| (2,3728) | 1:A:55:ASN:H | 1:A:54:VAL:H | 9 | 0.15 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 3 | 0.15 |
| (2,3526) | 1:A:5:SER:H | 1:A:6:GLU:HA | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 9 | 0.15 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 9 | 0.15 |
| (2,3385) | 1:A:37:VAL:HG12 | 2:B:113:GLY:HA2 | 1 | 0.15 |
| (2,3385) | 1:A:37:VAL:HG13 | 2:B:113:GLY:HA2 | 1 | 0.15 |
| (2,3385) | 1:A:37:VAL:HG22 | 2:B:113:GLY:HA2 | 1 | 0.15 |
| (2,3385) | 1:A:37:VAL:HG21 | 2:B:113:GLY:HA2 | 1 | 0.15 |
| (2,3385) | 1:A:37:VAL:HG23 | 2:B:113:GLY:HA2 | 1 | 0.15 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB2 | 3 | 0.15 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB3 | 3 | 0.15 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB2 | 7 | 0.15 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB3 | 7 | 0.15 |
| (2,3347) | 1:A:15:ILE:HG22 | 2:B:101:MET:HE2 | 7 | 0.15 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE2 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE3 | 7 | 0.15 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE2 | 7 | 0.15 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE1 | 7 | 0.15 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE3 | 7 | 0.15 |
| (2,3331) | 1:A:14:LEU:HD13 | 2:B:159:ILE:HA | 7 | 0.15 |
| (2,3331) | 1:A:14:LEU:HD22 | 2:B:159:ILE:HA | 7 | 0.15 |
| (2,3331) | 1:A:14:LEU:HD21 | 2:B:159:ILE:HA | 7 | 0.15 |
| (2,3331) | 1:A:14:LEU:HD23 | 2:B:159:ILE:HA | 7 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 6 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 6 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 6 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 6 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 6 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 6 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 7 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 7 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 7 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 7 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 7 | 0.15 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 7 | 0.15 |
| (2,3284) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 7 | 0.15 |
| (2,3284) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 7 | 0.15 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 1 | 0.15 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 1 | 0.15 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 7 | 0.15 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 7 | 0.15 |
| (2,3237) | 2:B:161:LYS:HA | 2:B:161:LYS:HG2 | 5 | 0.15 |
| (2,3237) | 2:B:161:LYS:HA | 2:B:161:LYS:HG3 | 5 | 0.15 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 2 | 0.15 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 2 | 0.15 |
| (2,3232) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 2 | 0.15 |
| (2,3195) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 6 | 0.15 |
| (2,3195) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 6 | 0.15 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 6 | 0.15 |
| (2,3195) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 6 | 0.15 |
| (2,3173) | 2:B:154:VAL:HG22 | 2:B:151:ILE:HG12 | 8 | 0.15 |
| (2,3173) | 2:B:154:VAL:HG21 | 2:B:151:ILE:HG12 | 8 | 0.15 |
| (2,3173) | 2:B:154:VAL:HG23 | 2:B:151:ILE:HG12 | 8 | 0.15 |
| (2,3168) | 2:B:154:VAL:HG12 | 2:B:154:VAL:HA | 9 | 0.15 |
| (2,3168) | 2:B:154:VAL:HG13 | 2:B:154:VAL:HA | 9 | 0.15 |
| (2,3168) | 2:B:154:VAL:HG22 | 2:B:154:VAL:HA | 9 | 0.15 |
| (2,3168) | 2:B:154:VAL:HG21 | 2:B:154:VAL:HA | 9 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3148) | 2:B:151:ILE:HG22 | 2:B:151:ILE:HA | 10 | 0.15 |
| (2,3148) | 2:B:151:ILE:HG21 | 2:B:151:ILE:HA | 10 | 0.15 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG2 | 5 | 0.15 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG3 | 5 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 5 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 5 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 5 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 5 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 9 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 9 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 9 | 0.15 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 9 | 0.15 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 8 | 0.15 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 8 | 0.15 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG21 | 4 | 0.15 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG23 | 4 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG12 | 2:B:107:TYR:HD2 | 4 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG11 | 2:B:107:TYR:HD2 | 4 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG13 | 2:B:107:TYR:HD2 | 4 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD1 | 4 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD2 | 4 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HE2 | 4 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG21 | 2:B:107:TYR:HD2 | 4 | 0.15 |
| (2,3054) | 2:B:142:VAL:HG23 | 2:B:107:TYR:HD2 | 4 | 0.15 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 8 | 0.15 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 8 | 0.15 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 8 | 0.15 |
| (2,3050) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 8 | 0.15 |
| (2,2976) | 2:B:134:ALA:HB2 | 2:B:135:ASP:HB3 | 3 | 0.15 |
| (2,2976) | 2:B:134:ALA:HB1 | 2:B:135:ASP:HB3 | 3 | 0.15 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB2 | 3 | 0.15 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB3 | 3 | 0.15 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 1 | 0.15 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 1 | 0.15 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 1 | 0.15 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 4 | 0.15 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 4 | 0.15 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 4 | 0.15 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 2 | 0.15 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 2 | 0.15 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 7 | 0.15 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 5 | 0.15 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 5 | 0.15 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 5 | 0.15 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 6 | 0.15 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 6 | 0.15 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 6 | 0.15 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 9 | 0.15 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 9 | 0.15 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 9 | 0.15 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 10 | 0.15 |
| (2,2775) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 10 | 0.15 |
| (2,2775) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 10 | 0.15 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 4 | 0.15 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 4 | 0.15 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 4 | 0.15 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 4 | 0.15 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 8 | 0.15 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 8 | 0.15 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 8 | 0.15 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 8 | 0.15 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 8 | 0.15 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 8 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 2 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 2 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 5 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 5 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 6 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 6 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 7 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 7 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 8 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 8 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 9 | 0.15 |
| (2,2701) | 2:B:109:LEU:HB2 | 2:B:109:LEU:HB3 | 9 | 0.15 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 6 | 0.15 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 6 | 0.15 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 9 | 0.15 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 9 | 0.15 |
| (2,2589) | 1:A:62:ASN:HB3 | 1:A:43:TRP:HZ2 | 1 | 0.15 |
| (2,2589) | 1:A:62:ASN:HB2 | 1:A:43:TRP:HZ2 | 1 | 0.15 |
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 2 | 0.15 |
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 5 | 0.15 |
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 5 | 0.15 |
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 7 | 0.15 |
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 7 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 1 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 1 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 1 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 2 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 2 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 2 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 3 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 3 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 3 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 4 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 4 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 4 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 5 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 5 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 5 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 7 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 7 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 7 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 8 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 8 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 8 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 9 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 9 | 0.15 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 9 | 0.15 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 4 | 0.15 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 4 | 0.15 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 4 | 0.15 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 4 | 0.15 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 4 | 0.15 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 4 | 0.15 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 3 | 0.15 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 3 | 0.15 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG2 | 1 | 0.15 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG3 | 1 | 0.15 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG2 | 2 | 0.15 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG3 | 2 | 0.15 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG22 | 6 | 0.15 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG21 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG23 | 6 | 0.15 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 5 | 0.15 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 5 | 0.15 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 9 | 0.15 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 9 | 0.15 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 10 | 0.15 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 10 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 9 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 9 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 9 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 9 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 9 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 9 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 10 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 10 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 10 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 10 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 10 | 0.15 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 10 | 0.15 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 10 | 0.15 |
| (2,2328) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 10 | 0.15 |
| (2,2328) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 10 | 0.15 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD12 | 6 | 0.15 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD11 | 6 | 0.15 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD13 | 6 | 0.15 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 4 | 0.15 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 4 | 0.15 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 4 | 0.15 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG22 | 9 | 0.15 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG21 | 9 | 0.15 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG23 | 9 | 0.15 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD21 | 9 | 0.15 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD23 | 9 | 0.15 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG22 | 9 | 0.15 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG21 | 9 | 0.15 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG23 | 9 | 0.15 |
| (2,2098) | 1:A:10:ILE:HD13 | 1:A:7:LEU:HG | 10 | 0.15 |
| (2,2098) | 1:A:10:ILE:HD12 | 1:A:7:LEU:HG | 10 | 0.15 |
| (2,2098) | 1:A:10:ILE:HD11 | 1:A:7:LEU:HG | 10 | 0.15 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 10 | 0.15 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 10 | 0.15 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 10 | 0.15 |
| (2,2015) | 2:B:166:PRO:HG2 | 2:B:166:PRO:HA | 7 | 0.15 |
| (2,2015) | 2:B:166:PRO:HG3 | 2:B:166:PRO:HA | 7 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG12 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG13 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD2 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD3 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG12 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG13 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HD3 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:151:ILE:HG12 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HD3 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG12 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG13 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:155:ILE:HG12 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG12 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG13 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HD3 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG12 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG13 | 5 | 0.15 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HD3 | 5 | 0.15 |
| (2,1876) | 2:B:143:ILE:HG21 | 2:B:147:ASN:HB2 | 6 | 0.15 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB2 | 6 | 0.15 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB3 | 6 | 0.15 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB2 | 2 | 0.15 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB3 | 2 | 0.15 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB2 | 8 | 0.15 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB3 | 8 | 0.15 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE2 | 9 | 0.15 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE3 | 9 | 0.15 |
| (2,1716) | 2:B:121:LYS:HG3 | 2:B:121:LYS:HE3 | 9 | 0.15 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG2 | 3 | 0.15 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG3 | 3 | 0.15 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG2 | 3 | 0.15 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG3 | 3 | 0.15 |
| (2,1614) | 2:B:101:MET:HE1 | 1:A:14:LEU:HB2 | 6 | 0.15 |
| (2,1614) | 2:B:101:MET:HE3 | 1:A:14:LEU:HB2 | 6 | 0.15 |
| (2,1614) | 2:B:101:MET:HE2 | 1:A:14:LEU:HB2 | 6 | 0.15 |
| (2,159) | 1:A:63:VAL:H | 1:A:62:ASN:HB2 | 3 | 0.15 |
| (2,159) | 1:A:63:VAL:H | 1:A:62:ASN:HB3 | 3 | 0.15 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 10 | 0.15 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 10 | 0.15 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD12 | 10 | 0.15 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD11 | 10 | 0.15 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD13 | 10 | 0.15 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD12 | 10 | 0.15 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD11 | 10 | 0.15 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD13 | 10 | 0.15 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD21 | 10 | 0.15 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD23 | 10 | 0.15 |
| (2,1393) | 1:A:24:THR:HG21 | 1:A:26:ASP:HB3 | 1 | 0.15 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB2 | 1 | 0.15 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB3 | 1 | 0.15 |
| (2,1393) | 1:A:24:THR:HG23 | 1:A:26:ASP:HB3 | 1 | 0.15 |
| (2,1393) | 1:A:24:THR:HG21 | 1:A:26:ASP:HB3 | 8 | 0.15 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB2 | 8 | 0.15 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB3 | 8 | 0.15 |
| (2,1393) | 1:A:24:THR:HG23 | 1:A:26:ASP:HB3 | 8 | 0.15 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 4 | 0.15 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 4 | 0.15 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 4 | 0.15 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 4 | 0.15 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 8 | 0.15 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 8 | 0.15 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 8 | 0.15 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB3 | 9 | 0.15 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB2 | 9 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD22 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD21 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD23 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD22 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD21 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD23 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD22 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD21 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD23 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD22 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD21 | 6 | 0.15 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD23 | 6 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 1 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 1 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 1 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 2 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 2 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 3 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 3 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 3 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 6 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 6 | 0.15 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 6 | 0.15 |
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 4 | 0.15 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 4 | 0.15 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 4 | 0.15 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 4 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 5 | 0.15 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 5 | 0.15 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 2 | 0.15 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 2 | 0.15 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 6 | 0.15 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 6 | 0.15 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 7 | 0.15 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 7 | 0.15 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 7 | 0.15 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 9 | 0.15 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 9 | 0.15 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 9 | 0.15 |
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 5 | 0.15 |
| (2,1084) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 5 | 0.15 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 9 | 0.15 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 9 | 0.15 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG2 | 4 | 0.15 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG3 | 4 | 0.15 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 6 | 0.15 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 6 | 0.15 |
| (2,1042) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 6 | 0.15 |
| (1,82) | 2:B:129:SER:H | 2:B:125:LYS:O | 1 | 0.15 |
| (1,82) | 2:B:129:SER:H | 2:B:125:LYS:O | 2 | 0.15 |
| (1,81) | 2:B:129:SER:N | 2:B:125:LYS:O | 2 | 0.15 |
| (1,68) | 2:B:113:GLY:H | 2:B:109:LEU:O | 1 | 0.15 |
| (1,68) | 2:B:113:GLY:H | 2:B:109:LEU:O | 3 | 0.15 |
| (1,67) | 2:B:113:GLY:N | 2:B:109:LEU:O | 1 | 0.15 |
| (1,67) | 2:B:113:GLY:N | 2:B:109:LEU:O | 3 | 0.15 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 3 | 0.15 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 3 | 0.15 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 6 | 0.15 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 7 | 0.15 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 7 | 0.15 |
| (1,25) | 1:A:28:ILE:N | 1:A:24:THR:O | 2 | 0.15 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 3 | 0.15 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 10 | 0.15 |
| (1,19) | 1:A:16:LEU:N | 1:A:12:SER:O | 6 | 0.15 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 8 | 0.14 |
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 8 | 0.14 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 8 | 0.14 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 8 | 0.14 |
| (2,850) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 8 | 0.14 |
| (2,850) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 8 | 0.14 |
| (2,792) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 5 | 0.14 |
| (2,792) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 5 | 0.14 |
| (2,735) | 1:A:59:LEU:HA | 1:A:59:LEU:HD22 | 5 | 0.14 |
| (2,735) | 1:A:59:LEU:HA | 1:A:59:LEU:HD21 | 5 | 0.14 |
| (2,735) | 1:A:59:LEU:HA | 1:A:59:LEU:HD22 | 10 | 0.14 |
| (2,735) | 1:A:59:LEU:HA | 1:A:59:LEU:HD21 | 10 | 0.14 |
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG12 | 1 | 0.14 |
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG11 | 1 | 0.14 |
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG13 | 1 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 1 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 1 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 1 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 1 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 1 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 4 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 4 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 4 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 4 | 0.14 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 4 | 0.14 |
| (2,695) | 1:A:51:LEU:HD12 | 1:A:48:ALA:HA | 3 | 0.14 |
| (2,695) | 1:A:51:LEU:HD11 | 1:A:48:ALA:HA | 3 | 0.14 |
| (2,695) | 1:A:51:LEU:HD13 | 1:A:48:ALA:HA | 3 | 0.14 |
| (2,671) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 6 | 0.14 |
| (2,671) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 6 | 0.14 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG12 | 5 | 0.14 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG11 | 5 | 0.14 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG13 | 5 | 0.14 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG21 | 5 | 0.14 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG12 | 10 | 0.14 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG11 | 10 | 0.14 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG13 | 10 | 0.14 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG21 | 10 | 0.14 |
| (2,587) | 1:A:37:VAL:HG12 | 2:B:112:LEU:HD23 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD22 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD21 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD21 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 5 | 0.14 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 5 | 0.14 |
| (2,558) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 2 | 0.14 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 2 | 0.14 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 2 | 0.14 |
| (2,522) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 9 | 0.14 |
| (2,522) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 9 | 0.14 |
| (2,498) | 1:A:25:GLU:HG2 | 1:A:48:ALA:HB1 | 7 | 0.14 |
| (2,498) | 1:A:25:GLU:HG2 | 1:A:48:ALA:HB3 | 7 | 0.14 |
| (2,498) | 1:A:25:GLU:HG3 | 1:A:48:ALA:HB1 | 7 | 0.14 |
| (2,498) | 1:A:25:GLU:HG3 | 1:A:48:ALA:HB3 | 7 | 0.14 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG22 | 2 | 0.14 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG21 | 2 | 0.14 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG23 | 2 | 0.14 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG22 | 5 | 0.14 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG21 | 5 | 0.14 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG23 | 5 | 0.14 |
| (2,4512) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 5 | 0.14 |
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 1 | 0.14 |
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 3 | 0.14 |
| (2,4338) | 1:A:39:VAL:HB | 1:A:38:ASN:HA | 8 | 0.14 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 1 | 0.14 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 3 | 0.14 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 7 | 0.14 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 10 | 0.14 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 3 | 0.14 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 4 | 0.14 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 6 | 0.14 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 8 | 0.14 |
| (2,4247) | 1:A:14:LEU:HG | 1:A:14:LEU:HA | 9 | 0.14 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 1 | 0.14 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 10 | 0.14 |
| (2,4136) | 1:A:22:THR:HA | 1:A:22:THR:HB | 4 | 0.14 |
| (2,4104) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 5 | 0.14 |
| (2,4006) | 2:B:169:GLY:H | 2:B:168:GLY:H | 7 | 0.14 |
| (2,4001) | 2:B:164:SER:H | 2:B:163:ALA:HA | 2 | 0.14 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 5 | 0.14 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 5 | 0.14 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 9 | 0.14 |
| (2,3999) | 2:B:160:GLY:H | 2:B:162:LEU:H | 7 | 0.14 |
| (2,3852) | 2:B:124:LYS:H | 2:B:125:LYS:HA | 5 | 0.14 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB2 | 9 | 0.14 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB3 | 9 | 0.14 |
| (2,3783) | 2:B:108:LEU:H | 2:B:108:LEU:HG | 1 | 0.14 |
| (2,3762) | 1:A:43:TRP:HE1 | 1:A:40:GLU:H | 10 | 0.14 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 1 | 0.14 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 4 | 0.14 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 1 | 0.14 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 5 | 0.14 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 6 | 0.14 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 10 | 0.14 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG12 | 9 | 0.14 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG13 | 9 | 0.14 |
| (2,3509) | 2:B:159:ILE:HG23 | 1:A:10:ILE:HG13 | 9 | 0.14 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG12 | 9 | 0.14 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG13 | 9 | 0.14 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG12 | 3 | 0.14 |
| (2,3443) | 2:B:110:ALA:HB2 | 1:A:37:VAL:HG13 | 3 | 0.14 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG12 | 3 | 0.14 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG11 | 3 | 0.14 |
| (2,3443) | 2:B:110:ALA:HB1 | 1:A:37:VAL:HG13 | 3 | 0.14 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG12 | 3 | 0.14 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG11 | 3 | 0.14 |
| (2,3443) | 2:B:110:ALA:HB3 | 1:A:37:VAL:HG13 | 3 | 0.14 |
| (2,3416) | 2:B:101:MET:HE2 | 1:A:17:HIS:HD2 | 9 | 0.14 |
| (2,3416) | 2:B:101:MET:HE1 | 1:A:17:HIS:HD2 | 9 | 0.14 |
| (2,3416) | 2:B:101:MET:HE3 | 1:A:17:HIS:HD2 | 9 | 0.14 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB2 | 2 | 0.14 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB3 | 2 | 0.14 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB2 | 2 | 0.14 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB3 | 2 | 0.14 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB2 | 6 | 0.14 |
| (2,3408) | 1:A:60:ILE:HD12 | 2:B:157:GLN:HB3 | 6 | 0.14 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB2 | 6 | 0.14 |
| (2,3408) | 1:A:60:ILE:HD13 | 2:B:157:GLN:HB3 | 6 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD12 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD11 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG11 | 2:B:109:LEU:HD13 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD12 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD11 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG13 | 2:B:109:LEU:HD13 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG21 | 2:B:109:LEU:HD13 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD12 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD11 | 8 | 0.14 |
| (2,3388) | 1:A:37:VAL:HG12 | 2:B:109:LEU:HD13 | 8 | 0.14 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 5 | 0.14 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 5 | 0.14 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 5 | 0.14 |
| (2,3306) | 1:A:4:VAL:HG11 | 2:B:112:LEU:HG | 1 | 0.14 |
| (2,3306) | 1:A:4:VAL:HG22 | 2:B:112:LEU:HG | 1 | 0.14 |
| (2,3306) | 1:A:4:VAL:HG21 | 2:B:112:LEU:HG | 1 | 0.14 |
| (2,3306) | 1:A:4:VAL:HG23 | 2:B:112:LEU:HG | 1 | 0.14 |
| (2,3305) | 1:A:4:VAL:HG11 | 2:B:112:LEU:HA | 9 | 0.14 |
| (2,3305) | 1:A:4:VAL:HG22 | 2:B:112:LEU:HA | 9 | 0.14 |
| (2,3305) | 1:A:4:VAL:HG21 | 2:B:112:LEU:HA | 9 | 0.14 |
| (2,3305) | 1:A:4:VAL:HG23 | 2:B:112:LEU:HA | 9 | 0.14 |
| (2,3296) | 1:A:1:MET:HE1 | 2:B:156:ALA:HA | 6 | 0.14 |
| (2,3296) | 1:A:1:MET:HE3 | 2:B:156:ALA:HA | 6 | 0.14 |
| (2,3296) | 1:A:1:MET:HE2 | 2:B:156:ALA:HA | 6 | 0.14 |
| (2,3261) | 2:B:163:ALA:HB2 | 2:B:163:ALA:H | 8 | 0.14 |
| (2,3261) | 2:B:163:ALA:HB3 | 2:B:163:ALA:H | 8 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD12 | 1 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD11 | 1 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD13 | 1 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD12 | 7 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD11 | 7 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD13 | 7 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD12 | 10 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD11 | 10 | 0.14 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD13 | 10 | 0.14 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG21 | 9 | 0.14 |
| (2,317) | 2:B:154:VAL:H | 2:B:154:VAL:HG23 | 9 | 0.14 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG2 | 9 | 0.14 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG3 | 9 | 0.14 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD12 | 6 | 0.14 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD13 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD22 | 6 | 0.14 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD21 | 6 | 0.14 |
| (2,3111) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB2 | 6 | 0.14 |
| (2,3111) | 2:B:146:LEU:HD21 | 2:B:107:TYR:HB3 | 6 | 0.14 |
| (2,3111) | 2:B:104:VAL:HA | 2:B:146:LEU:HD23 | 6 | 0.14 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 7 | 0.14 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 7 | 0.14 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 7 | 0.14 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 7 | 0.14 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD12 | 8 | 0.14 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD11 | 8 | 0.14 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD13 | 8 | 0.14 |
| (2,3103) | 2:B:146:LEU:HA | 2:B:146:LEU:HD22 | 8 | 0.14 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 9 | 0.14 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 9 | 0.14 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 9 | 0.14 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB1 | 3 | 0.14 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB3 | 3 | 0.14 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 9 | 0.14 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 9 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 2 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 2 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 2 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 9 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 9 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 9 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 10 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 10 | 0.14 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 10 | 0.14 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 6 | 0.14 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 6 | 0.14 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 6 | 0.14 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 6 | 0.14 |
| (2,2716) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 9 | 0.14 |
| (2,2716) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 9 | 0.14 |
| (2,2716) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 9 | 0.14 |
| (2,2716) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 9 | 0.14 |
| (2,2715) | 2:B:110:ALA:HB2 | 2:B:115:ASN:H | 2 | 0.14 |
| (2,2715) | 2:B:110:ALA:HB1 | 2:B:115:ASN:H | 2 | 0.14 |
| (2,2715) | 2:B:110:ALA:HB3 | 2:B:115:ASN:H | 2 | 0.14 |
| (2,2610) | 1:A:47:PHE:HE2 | 1:A:43:TRP:HZ2 | 3 | 0.14 |
| (2,2610) | 1:A:47:PHE:HE1 | 1:A:43:TRP:HZ2 | 3 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,2607) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD2 | 1 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD2 | 1 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD1 | 1 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD11 | 1:A:47:PHE:HD1 | 1 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD1 | 1 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD13 | 1:A:47:PHE:HD1 | 1 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD23 | 1:A:47:PHE:HD2 | 1 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD13 | 1:A:47:PHE:HD2 | 1 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD23 | 1:A:47:PHE:HD1 | 1 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD2 | 9 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD2 | 9 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD1 | 9 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD11 | 1:A:47:PHE:HD1 | 9 | 0.14 |
| (2,2607) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD1 | 9 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD13 | 1:A:47:PHE:HD1 | 9 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD23 | 1:A:47:PHE:HD2 | 9 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD13 | 1:A:47:PHE:HD2 | 9 | 0.14 |
| (2,2607) | 1:A:59:LEU:HD23 | 1:A:47:PHE:HD1 | 9 | 0.14 |
| (2,2589) | 1:A:62:ASN:HB3 | 1:A:43:TRP:HZ2 | 6 | 0.14 |
| (2,2589) | 1:A:62:ASN:HB2 | 1:A:43:TRP:HZ2 | 6 | 0.14 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 3 | 0.14 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 3 | 0.14 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 7 | 0.14 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 7 | 0.14 |
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 3 | 0.14 |
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 3 | 0.14 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 6 | 0.14 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 6 | 0.14 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 6 | 0.14 |
| (2,2480) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 10 | 0.14 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 10 | 0.14 |
| (2,2480) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 10 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 1 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 1 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 2 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 2 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 4 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 4 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 5 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 5 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 6 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 7 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 7 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 8 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 8 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 9 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 9 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 10 | 0.14 |
| (2,2452) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 10 | 0.14 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 6 | 0.14 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 6 | 0.14 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG2 | 5 | 0.14 |
| (2,242) | 2:B:125:LYS:H | 2:B:125:LYS:HG3 | 5 | 0.14 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG22 | 8 | 0.14 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG21 | 8 | 0.14 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG23 | 8 | 0.14 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 3 | 0.14 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 3 | 0.14 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 4 | 0.14 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 4 | 0.14 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 6 | 0.14 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 6 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 8 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 8 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 8 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 8 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 8 | 0.14 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 8 | 0.14 |
| (2,2286) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 9 | 0.14 |
| (2,2286) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 9 | 0.14 |
| (2,2285) | 1:A:28:ILE:HA | 1:A:31:LEU:HD22 | 4 | 0.14 |
| (2,2285) | 1:A:28:ILE:HA | 1:A:31:LEU:HD11 | 4 | 0.14 |
| (2,2238) | 1:A:23:VAL:HG12 | 1:A:51:LEU:H | 2 | 0.14 |
| (2,2238) | 1:A:23:VAL:HG11 | 1:A:51:LEU:H | 2 | 0.14 |
| (2,2238) | 1:A:23:VAL:HG13 | 1:A:51:LEU:H | 2 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 8 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 8 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 8 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 9 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 9 | 0.14 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 9 | 0.14 |
| (2,2204) | 1:A:20:GLU:HG2 | 1:A:19:ASP:H | 7 | 0.14 |
| (2,2204) | 1:A:20:GLU:HG3 | 1:A:19:ASP:H | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG22 | 7 | 0.14 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG21 | 7 | 0.14 |
| (2,2181) | 1:A:17:HIS:HB2 | 1:A:56:ILE:HG23 | 7 | 0.14 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD21 | 7 | 0.14 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:51:LEU:HD23 | 7 | 0.14 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG22 | 7 | 0.14 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG21 | 7 | 0.14 |
| (2,2181) | 1:A:17:HIS:HB3 | 1:A:56:ILE:HG23 | 7 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 1 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 1 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 1 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 7 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 7 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 7 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 8 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 8 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 8 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB3 | 2:B:167:ALA:HA | 10 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB2 | 2:B:167:ALA:HA | 10 | 0.14 |
| (2,2030) | 2:B:167:ALA:HB1 | 2:B:167:ALA:HA | 10 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 3 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 3 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 3 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 4 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 4 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 4 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 5 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 5 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 5 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 7 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 7 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 7 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 8 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 8 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 8 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 9 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 9 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 9 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 10 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 10 | 0.14 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 10 | 0.14 |
| (2,1988) | 2:B:161:LYS:HD2 | 2:B:161:LYS:HA | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1988) | 2:B:161:LYS:HD3 | 2:B:161:LYS:HA | 2 | 0.14 |
| (2,1905) | 2:B:147:ASN:HA | 2:B:147:ASN:HB2 | 4 | 0.14 |
| (2,1905) | 2:B:147:ASN:HA | 2:B:147:ASN:HB3 | 4 | 0.14 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 8 | 0.14 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 8 | 0.14 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 8 | 0.14 |
| (2,1864) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 8 | 0.14 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 2 | 0.14 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 2 | 0.14 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 4 | 0.14 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 4 | 0.14 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB2 | 1 | 0.14 |
| (2,1826) | 2:B:136:ASP:HA | 2:B:136:ASP:HB3 | 1 | 0.14 |
| (2,1758) | 2:B:126:ILE:HA | 2:B:125:LYS:HD2 | 9 | 0.14 |
| (2,1758) | 2:B:126:ILE:HA | 2:B:125:LYS:HD3 | 9 | 0.14 |
| (2,1700) | 2:B:139:LEU:HD12 | 2:B:120:ALA:HA | 6 | 0.14 |
| (2,1700) | 2:B:139:LEU:HD11 | 2:B:120:ALA:HA | 6 | 0.14 |
| (2,1700) | 2:B:139:LEU:HD22 | 2:B:120:ALA:HA | 6 | 0.14 |
| (2,1700) | 2:B:139:LEU:HD23 | 2:B:120:ALA:HA | 6 | 0.14 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG2 | 8 | 0.14 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG3 | 8 | 0.14 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG2 | 8 | 0.14 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG3 | 8 | 0.14 |
| (2,162) | 1:A:65:ALA:H | 1:A:65:ALA:HB1 | 8 | 0.14 |
| (2,162) | 1:A:65:ALA:H | 1:A:65:ALA:HB3 | 8 | 0.14 |
| (2,1614) | 2:B:101:MET:HE1 | 1:A:14:LEU:HB2 | 1 | 0.14 |
| (2,1614) | 2:B:101:MET:HE3 | 1:A:14:LEU:HB2 | 1 | 0.14 |
| (2,1614) | 2:B:101:MET:HE2 | 1:A:14:LEU:HB2 | 1 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 1 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 1 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 1 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 2 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 2 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 2 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 3 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 3 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 3 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 4 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 4 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 4 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 5 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 5 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 7 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 7 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 7 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 8 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 8 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 8 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 9 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 9 | 0.14 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 9 | 0.14 |
| (2,1510) | 1:A:28:ILE:HD12 | 1:A:44:PRO:HA | 9 | 0.14 |
| (2,1510) | 1:A:28:ILE:HD13 | 1:A:44:PRO:HA | 9 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 1 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 1 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 2 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 2 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 3 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 3 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 4 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 4 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 5 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 5 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 6 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 6 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 7 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 7 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 8 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 8 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 9 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 9 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 10 | 0.14 |
| (2,1508) | 1:A:43:TRP:HB2 | 1:A:43:TRP:HB3 | 10 | 0.14 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG12 | 4 | 0.14 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG11 | 4 | 0.14 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG13 | 4 | 0.14 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG23 | 4 | 0.14 |
| (2,1391) | 1:A:24:THR:HG21 | 1:A:27:LYS:HE3 | 9 | 0.14 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE2 | 9 | 0.14 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE3 | 9 | 0.14 |
| (2,1391) | 1:A:24:THR:HG23 | 1:A:27:LYS:HE3 | 9 | 0.14 |
| (2,1391) | 1:A:24:THR:HG21 | 1:A:27:LYS:HE3 | 10 | 0.14 |
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE2 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1391) | 1:A:24:THR:HG22 | 1:A:27:LYS:HE3 | 10 | 0.14 |
| (2,1391) | 1:A:24:THR:HG23 | 1:A:27:LYS:HE3 | 10 | 0.14 |
| (2,135) | 1:A:51:LEU:H | 1:A:51:LEU:HD12 | 6 | 0.14 |
| (2,135) | 1:A:51:LEU:H | 1:A:51:LEU:HD11 | 6 | 0.14 |
| (2,135) | 1:A:51:LEU:H | 1:A:51:LEU:HD13 | 6 | 0.14 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 6 | 0.14 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 6 | 0.14 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 6 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD22 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD21 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD23 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD22 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD21 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD23 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD22 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD21 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD23 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD22 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD21 | 10 | 0.14 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD23 | 10 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 4 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 4 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 4 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 5 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 5 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 5 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 7 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 7 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 7 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 8 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 8 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 8 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 9 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 9 | 0.14 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 9 | 0.14 |
| (2,1186) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 6 | 0.14 |
| (2,1186) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 6 | 0.14 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 6 | 0.14 |
| (2,1186) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 6 | 0.14 |
| (2,1162) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 8 | 0.14 |
| (2,1162) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 8 | 0.14 |
| (2,1162) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 1 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 1 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 4 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 4 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 6 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 6 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 7 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 7 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 8 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 8 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 9 | 0.14 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 9 | 0.14 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 6 | 0.14 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 6 | 0.14 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 6 | 0.14 |
| (2,1034) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD1 | 5 | 0.14 |
| (2,1034) | 2:B:134:ALA:HB2 | 2:B:103:TYR:HD2 | 5 | 0.14 |
| (2,1034) | 2:B:134:ALA:HB1 | 2:B:103:TYR:HD2 | 5 | 0.14 |
| (2,1034) | 2:B:134:ALA:HB3 | 2:B:103:TYR:HD2 | 5 | 0.14 |
| (1,91) | 2:B:144:SER:N | 2:B:140:ASN:O | 2 | 0.14 |
| (1,87) | 2:B:142:VAL:N | 2:B:138:ARG:O | 9 | 0.14 |
| (1,75) | 2:B:126:ILE:N | 2:B:122:ASP:O | 3 | 0.14 |
| (1,75) | 2:B:126:ILE:N | 2:B:122:ASP:O | 7 | 0.14 |
| (1,55) | 2:B:107:TYR:N | 2:B:103:TYR:O | 8 | 0.14 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 7 | 0.14 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 9 | 0.14 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 10 | 0.14 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 5 | 0.14 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 9 | 0.14 |
| (1,32) | 1:A:31:LEU:H | 1:A:27:LYS:O | 4 | 0.14 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 9 | 0.14 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 10 | 0.14 |
| (1,25) | 1:A:28:ILE:N | 1:A:24:THR:O | 6 | 0.14 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 4 | 0.14 |
| (1,19) | 1:A:16:LEU:N | 1:A:12:SER:O | 8 | 0.14 |
| (2,919) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 7 | 0.13 |
| (2,919) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 7 | 0.13 |
| (2,919) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 7 | 0.13 |
| (2,919) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 10 | 0.13 |
| (2,919) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 10 | 0.13 |
| (2,919) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 10 | 0.13 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 4 | 0.13 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 6 | 0.13 |
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 6 | 0.13 |
| (2,829) | 2:B:108:LEU:HD12 | 2:B:154:VAL:HB | 1 | 0.13 |
| (2,829) | 2:B:108:LEU:HD13 | 2:B:154:VAL:HB | 1 | 0.13 |
| (2,794) | 2:B:104:VAL:HG22 | 2:B:105:ALA:HA | 5 | 0.13 |
| (2,794) | 2:B:104:VAL:HG21 | 2:B:105:ALA:HA | 5 | 0.13 |
| (2,794) | 2:B:104:VAL:HG23 | 2:B:105:ALA:HA | 5 | 0.13 |
| (2,794) | 2:B:104:VAL:HG11 | 2:B:105:ALA:HA | 5 | 0.13 |
| (2,790) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD21 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG12 | 2:B:146:LEU:HD23 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG11 | 2:B:146:LEU:HD21 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD22 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG13 | 2:B:146:LEU:HD21 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD13 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD22 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD21 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG22 | 2:B:146:LEU:HD23 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD21 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG21 | 2:B:146:LEU:HD23 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD22 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD21 | 8 | 0.13 |
| (2,790) | 2:B:104:VAL:HG23 | 2:B:146:LEU:HD23 | 8 | 0.13 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE2 | 10 | 0.13 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE1 | 10 | 0.13 |
| (2,776) | 1:A:14:LEU:HA | 2:B:101:MET:HE3 | 10 | 0.13 |
| (2,739) | 1:A:59:LEU:HD12 | 1:A:56:ILE:HA | 4 | 0.13 |
| (2,739) | 1:A:59:LEU:HD11 | 1:A:56:ILE:HA | 4 | 0.13 |
| (2,739) | 1:A:59:LEU:HD13 | 1:A:56:ILE:HA | 4 | 0.13 |
| (2,739) | 1:A:59:LEU:HD21 | 1:A:56:ILE:HA | 4 | 0.13 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 7 | 0.13 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 7 | 0.13 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 7 | 0.13 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 7 | 0.13 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 7 | 0.13 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB2 | 2 | 0.13 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB3 | 2 | 0.13 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB2 | 5 | 0.13 |
| (2,70) | 1:A:26:ASP:H | 1:A:25:GLU:HB3 | 5 | 0.13 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 1 | 0.13 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 1 | 0.13 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD13 | 7 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD22 | 7 | 0.13 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD21 | 7 | 0.13 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD23 | 7 | 0.13 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 8 | 0.13 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 8 | 0.13 |
| (2,587) | 1:A:37:VAL:HG12 | 2:B:112:LEU:HD23 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD22 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD21 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HD23 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HD23 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD22 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD21 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HD23 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD22 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD21 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HD23 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD22 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD21 | 10 | 0.13 |
| (2,587) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HD23 | 10 | 0.13 |
| (2,571) | 1:A:35:ALA:HA | 2:B:126:ILE:HG12 | 3 | 0.13 |
| (2,571) | 1:A:35:ALA:HA | 2:B:126:ILE:HG13 | 3 | 0.13 |
| (2,560) | 1:A:33:LYS:HA | 1:A:33:LYS:HG2 | 10 | 0.13 |
| (2,560) | 1:A:33:LYS:HA | 1:A:33:LYS:HG3 | 10 | 0.13 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG22 | 10 | 0.13 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG21 | 10 | 0.13 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG23 | 10 | 0.13 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 4 | 0.13 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 8 | 0.13 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 3 | 0.13 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 8 | 0.13 |
| (2,4520) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 3 | 0.13 |
| (2,4520) | 2:B:145:GLU:HG2 | 2:B:145:GLU:H | 7 | 0.13 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 1 | 0.13 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 3 | 0.13 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 4 | 0.13 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 5 | 0.13 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 7 | 0.13 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 8 | 0.13 |
| (2,4458) | 2:B:125:LYS:HA | 2:B:125:LYS:HB3 | 4 | 0.13 |
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 2 | 0.13 |
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 5 | 0.13 |
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 10 | 0.13 |
| (2,4341) | 1:A:41:PRO:HA | 1:A:39:VAL:H | 2 | 0.13 |
| (2,4341) | 1:A:41:PRO:HA | 1:A:39:VAL:H | 6 | 0.13 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD12 | 5 | 0.13 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD11 | 5 | 0.13 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD13 | 5 | 0.13 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD21 | 5 | 0.13 |
| (2,4282) | 1:A:22:THR:HA | 1:A:23:VAL:HB | 9 | 0.13 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 4 | 0.13 |
| (2,4136) | 1:A:22:THR:HA | 1:A:22:THR:HB | 5 | 0.13 |
| (2,4136) | 1:A:22:THR:HA | 1:A:22:THR:HB | 9 | 0.13 |
| (2,4098) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 1 | 0.13 |
| (2,4098) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 2 | 0.13 |
| (2,4046) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 4 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 1 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 1 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 2 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 2 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 3 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 3 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 4 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 4 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 5 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 5 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 6 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 6 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 7 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 7 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 8 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 8 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 9 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 9 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.13 |
| (2,402) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.13 |
| (2,4001) | 2:B:164:SER:H | 2:B:163:ALA:HA | 1 | 0.13 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 10 | 0.13 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 10 | 0.13 |
| (2,3999) | 2:B:160:GLY:H | 2:B:162:LEU:H | 10 | 0.13 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 2 | 0.13 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 7 | 0.13 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 4 | 0.13 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 6 | 0.13 |
| (2,3528) | 1:A:5:SER:H | 1:A:3:SER:HA | 8 | 0.13 |
| (2,3492) | 2:B:152:GLU:HG2 | 1:A:7:LEU:HB3 | 8 | 0.13 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB2 | 8 | 0.13 |
| (2,3492) | 2:B:152:GLU:HG3 | 1:A:7:LEU:HB3 | 8 | 0.13 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG22 | 1 | 0.13 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG21 | 1 | 0.13 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG23 | 1 | 0.13 |
| (2,3488) | 2:B:152:GLU:HB3 | 1:A:4:VAL:HG21 | 1 | 0.13 |
| (2,3488) | 2:B:152:GLU:HB3 | 1:A:4:VAL:HG23 | 1 | 0.13 |
| (2,3430) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 4 | 0.13 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 4 | 0.13 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 4 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 7 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 7 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 7 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 7 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 7 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 7 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG22 | 8 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG21 | 8 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD11 | 2:B:159:ILE:HG23 | 8 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG21 | 8 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD13 | 2:B:159:ILE:HG23 | 8 | 0.13 |
| (2,3410) | 1:A:60:ILE:HD12 | 2:B:159:ILE:HG21 | 8 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 3 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 3 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 3 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 6 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 6 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 6 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 10 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 10 | 0.13 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 10 | 0.13 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB2 | 5 | 0.13 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB3 | 5 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD13 | 2:B:159:ILE:HA | 2 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD22 | 2:B:159:ILE:HA | 2 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD21 | 2:B:159:ILE:HA | 2 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD23 | 2:B:159:ILE:HA | 2 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD13 | 2:B:159:ILE:HA | 10 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD22 | 2:B:159:ILE:HA | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3331) | 1:A:14:LEU:HD21 | 2:B:159:ILE:HA | 10 | 0.13 |
| (2,3331) | 1:A:14:LEU:HD23 | 2:B:159:ILE:HA | 10 | 0.13 |
| (2,332) | 2:B:165:VAL:H | 2:B:164:SER:HB2 | 8 | 0.13 |
| (2,332) | 2:B:165:VAL:H | 2:B:164:SER:HB3 | 8 | 0.13 |
| (2,3287) | 2:B:166:PRO:HD2 | 2:B:166:PRO:HA | 7 | 0.13 |
| (2,3287) | 2:B:166:PRO:HD3 | 2:B:166:PRO:HA | 7 | 0.13 |
| (2,3270) | 2:B:165:VAL:HG12 | 2:B:161:LYS:HG2 | 8 | 0.13 |
| (2,3270) | 2:B:165:VAL:HG12 | 2:B:161:LYS:HG3 | 8 | 0.13 |
| (2,3270) | 2:B:165:VAL:HG11 | 2:B:161:LYS:HG2 | 8 | 0.13 |
| (2,3270) | 2:B:165:VAL:HG11 | 2:B:161:LYS:HG3 | 8 | 0.13 |
| (2,3270) | 2:B:165:VAL:HG13 | 2:B:161:LYS:HG3 | 8 | 0.13 |
| (2,3270) | 2:B:165:VAL:HG23 | 2:B:161:LYS:HG2 | 8 | 0.13 |
| (2,3270) | 2:B:165:VAL:HG23 | 2:B:161:LYS:HG3 | 8 | 0.13 |
| (2,3269) | 2:B:165:VAL:H | 2:B:165:VAL:HG22 | 9 | 0.13 |
| (2,3269) | 2:B:165:VAL:H | 2:B:165:VAL:HG21 | 9 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD12 | 2 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD11 | 2 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD13 | 2 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD12 | 4 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD11 | 4 | 0.13 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD13 | 4 | 0.13 |
| (2,3179) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 6 | 0.13 |
| (2,3179) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 6 | 0.13 |
| (2,3179) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 6 | 0.13 |
| (2,3179) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 6 | 0.13 |
| (2,3179) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 6 | 0.13 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG22 | 2 | 0.13 |
| (2,314) | 2:B:153:ASP:H | 2:B:151:ILE:HG21 | 2 | 0.13 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG21 | 2 | 0.13 |
| (2,314) | 2:B:153:ASP:H | 2:B:154:VAL:HG23 | 2 | 0.13 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG2 | 4 | 0.13 |
| (2,312) | 2:B:153:ASP:H | 2:B:152:GLU:HG3 | 4 | 0.13 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG22 | 10 | 0.13 |
| (2,3078) | 2:B:144:SER:H | 2:B:143:ILE:HG23 | 10 | 0.13 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG21 | 10 | 0.13 |
| (2,3070) | 2:B:120:ALA:H | 2:B:143:ILE:HG23 | 10 | 0.13 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 10 | 0.13 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 10 | 0.13 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 10 | 0.13 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 10 | 0.13 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG12 | 7 | 0.13 |
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG11 | 7 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3052) | 2:B:103:TYR:HB2 | 2:B:142:VAL:HG13 | 7 | 0.13 |
| (2,2872) | 2:B:125:LYS:HD2 | 2:B:125:LYS:HB2 | 4 | 0.13 |
| (2,2872) | 2:B:125:LYS:HD2 | 2:B:125:LYS:HB3 | 4 | 0.13 |
| (2,2872) | 2:B:125:LYS:HD3 | 2:B:125:LYS:HB2 | 4 | 0.13 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 6 | 0.13 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 6 | 0.13 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 6 | 0.13 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 4 | 0.13 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 4 | 0.13 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 1 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 1 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 1 | 0.13 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 2 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 2 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 2 | 0.13 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 3 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 3 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 3 | 0.13 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 4 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 4 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 4 | 0.13 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 7 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 7 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 7 | 0.13 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 8 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 8 | 0.13 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 8 | 0.13 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 9 | 0.13 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 9 | 0.13 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 9 | 0.13 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 9 | 0.13 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 6 | 0.13 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 6 | 0.13 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 6 | 0.13 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 7 | 0.13 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 7 | 0.13 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 7 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 1 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 1 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 1 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 1 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 5 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 5 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 5 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 10 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 10 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 10 | 0.13 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 10 | 0.13 |
| (2,2716) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 4 | 0.13 |
| (2,2716) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 4 | 0.13 |
| (2,2716) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 4 | 0.13 |
| (2,2716) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 4 | 0.13 |
| (2,2589) | 1:A:62:ASN:HB3 | 1:A:43:TRP:HZ2 | 7 | 0.13 |
| (2,2589) | 1:A:62:ASN:HB2 | 1:A:43:TRP:HZ2 | 7 | 0.13 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 1 | 0.13 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 1 | 0.13 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 4 | 0.13 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 4 | 0.13 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 7 | 0.13 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 7 | 0.13 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 1 | 0.13 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 1 | 0.13 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 8 | 0.13 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 8 | 0.13 |
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 4 | 0.13 |
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 4 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 1 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 1 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 2 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 2 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 3 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 3 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 4 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 4 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 5 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 5 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 6 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 6 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 7 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 7 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 8 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 8 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 9 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 10 | 0.13 |
| (2,2463) | 1:A:47:PHE:HB2 | 1:A:47:PHE:HB3 | 10 | 0.13 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 3 | 0.13 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 3 | 0.13 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 8 | 0.13 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 8 | 0.13 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 7 | 0.13 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 7 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 1 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 1 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 1 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 1 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 1 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 1 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 4 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 4 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 4 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 4 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 4 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 4 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 7 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 7 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 7 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 7 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 7 | 0.13 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 7 | 0.13 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD12 | 7 | 0.13 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD11 | 7 | 0.13 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD13 | 7 | 0.13 |
| (2,2238) | 1:A:23:VAL:HG12 | 1:A:51:LEU:H | 5 | 0.13 |
| (2,2238) | 1:A:23:VAL:HG11 | 1:A:51:LEU:H | 5 | 0.13 |
| (2,2238) | 1:A:23:VAL:HG13 | 1:A:51:LEU:H | 5 | 0.13 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 5 | 0.13 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 5 | 0.13 |
| (2,2057) | 1:A:4:VAL:HG12 | 2:B:112:LEU:HB3 | 1 | 0.13 |
| (2,2057) | 1:A:4:VAL:HG11 | 2:B:112:LEU:HB2 | 1 | 0.13 |
| (2,2057) | 1:A:4:VAL:HG11 | 2:B:112:LEU:HB3 | 1 | 0.13 |
| (2,2057) | 1:A:4:VAL:HG13 | 2:B:112:LEU:HB3 | 1 | 0.13 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 1 | 0.13 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 1 | 0.13 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 1 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 2 | 0.13 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 2 | 0.13 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 2 | 0.13 |
| (2,2004) | 2:B:163:ALA:HB1 | 2:B:163:ALA:HA | 6 | 0.13 |
| (2,2004) | 2:B:163:ALA:HB3 | 2:B:163:ALA:HA | 6 | 0.13 |
| (2,2004) | 2:B:163:ALA:HB2 | 2:B:163:ALA:HA | 6 | 0.13 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB3 | 7 | 0.13 |
| (2,1994) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HB3 | 7 | 0.13 |
| (2,1994) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HB2 | 7 | 0.13 |
| (2,1988) | 2:B:161:LYS:HD2 | 2:B:161:LYS:HA | 1 | 0.13 |
| (2,1988) | 2:B:161:LYS:HD3 | 2:B:161:LYS:HA | 1 | 0.13 |
| (2,1988) | 2:B:161:LYS:HD2 | 2:B:161:LYS:HA | 8 | 0.13 |
| (2,1988) | 2:B:161:LYS:HD3 | 2:B:161:LYS:HA | 8 | 0.13 |
| (2,1934) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 8 | 0.13 |
| (2,1934) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 8 | 0.13 |
| (2,1934) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 8 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG12 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:151:ILE:HG13 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD2 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HD3 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG12 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:151:ILE:HG13 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HD3 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:151:ILE:HG12 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HD3 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG12 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD21 | 2:B:151:ILE:HG13 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:155:ILE:HG12 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG12 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:151:ILE:HG13 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HD3 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG12 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:151:ILE:HG13 | 2 | 0.13 |
| (2,1898) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HD3 | 2 | 0.13 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 6 | 0.13 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 6 | 0.13 |
| (2,1814) | 2:B:133:GLU:HA | 2:B:133:GLU:HG3 | 3 | 0.13 |
| (2,1814) | 2:B:133:GLU:HA | 2:B:133:GLU:HG2 | 3 | 0.13 |
| (2,1758) | 2:B:126:ILE:HA | 2:B:125:LYS:HD2 | 1 | 0.13 |
| (2,1758) | 2:B:126:ILE:HA | 2:B:125:LYS:HD3 | 1 | 0.13 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 2 | 0.13 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 2 | 0.13 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 2 | 0.13 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 2 | 0.13 |
| (2,1659) | 2:B:111:ALA:HB2 | 2:B:151:ILE:HD12 | 9 | 0.13 |
| (2,1659) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD12 | 9 | 0.13 |
| (2,1659) | 2:B:111:ALA:HB1 | 2:B:151:ILE:HD11 | 9 | 0.13 |
| (2,1659) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD12 | 9 | 0.13 |
| (2,1659) | 2:B:111:ALA:HB3 | 2:B:151:ILE:HD11 | 9 | 0.13 |
| (2,1601) | 1:A:61:CYS:HA | 1:A:61:CYS:HB2 | 2 | 0.13 |
| (2,1601) | 1:A:61:CYS:HA | 1:A:61:CYS:HB3 | 2 | 0.13 |
| (2,1601) | 1:A:61:CYS:HA | 1:A:61:CYS:HB2 | 5 | 0.13 |
| (2,1601) | 1:A:61:CYS:HA | 1:A:61:CYS:HB3 | 5 | 0.13 |
| (2,1601) | 1:A:61:CYS:HA | 1:A:61:CYS:HB2 | 10 | 0.13 |
| (2,1601) | 1:A:61:CYS:HA | 1:A:61:CYS:HB3 | 10 | 0.13 |
| (2,1540) | 1:A:47:PHE:HA | 1:A:51:LEU:HD12 | 5 | 0.13 |
| (2,1540) | 1:A:47:PHE:HA | 1:A:51:LEU:HD13 | 5 | 0.13 |
| (2,1540) | 1:A:56:ILE:HA | 1:A:51:LEU:HD13 | 5 | 0.13 |
| (2,1540) | 1:A:56:ILE:HA | 1:A:51:LEU:HD23 | 5 | 0.13 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 6 | 0.13 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 6 | 0.13 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 6 | 0.13 |
| (2,1529) | 1:A:49:LYS:HD2 | 1:A:49:LYS:HG2 | 10 | 0.13 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG2 | 10 | 0.13 |
| (2,1529) | 1:A:49:LYS:HD3 | 1:A:49:LYS:HG3 | 10 | 0.13 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD12 | 5 | 0.13 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD11 | 5 | 0.13 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD13 | 5 | 0.13 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD12 | 5 | 0.13 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD11 | 5 | 0.13 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD13 | 5 | 0.13 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD21 | 5 | 0.13 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD23 | 5 | 0.13 |
| (2,1393) | 1:A:24:THR:HG21 | 1:A:26:ASP:HB3 | 2 | 0.13 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB2 | 2 | 0.13 |
| (2,1393) | 1:A:24:THR:HG22 | 1:A:26:ASP:HB3 | 2 | 0.13 |
| (2,1393) | 1:A:24:THR:HG23 | 1:A:26:ASP:HB3 | 2 | 0.13 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 1 | 0.13 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 1 | 0.13 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 8 | 0.13 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 8 | 0.13 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 8 | 0.13 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD22 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD21 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD23 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD22 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD21 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD23 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD22 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD21 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD23 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD22 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD21 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD23 | 4 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD22 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD21 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD23 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD22 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD21 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD23 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD22 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD21 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD23 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD22 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD21 | 8 | 0.13 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD23 | 8 | 0.13 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 10 | 0.13 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB1 | 10 | 0.13 |
| (2,1269) | 1:A:2:ALA:HA | 1:A:2:ALA:HB3 | 10 | 0.13 |
| (2,1266) | 1:A:1:MET:HG3 | 2:B:152:GLU:HG3 | 7 | 0.13 |
| (2,1266) | 1:A:1:MET:HG2 | 2:B:152:GLU:HG3 | 7 | 0.13 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD2 | 8 | 0.13 |
| (2,1240) | 2:B:165:VAL:HB | 2:B:166:PRO:HD3 | 8 | 0.13 |
| (2,1236) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 5 | 0.13 |
| (2,1236) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 5 | 0.13 |
| (2,1191) | 2:B:157:GLN:HB2 | 2:B:154:VAL:HA | 7 | 0.13 |
| (2,1191) | 2:B:157:GLN:HB3 | 2:B:154:VAL:HA | 7 | 0.13 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 6 | 0.13 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 6 | 0.13 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 6 | 0.13 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 4 | 0.13 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 4 | 0.13 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 9 | 0.13 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD13 | 7 | 0.13 |
| (2,1149) | 2:B:151:ILE:HB | 2:B:151:ILE:HD12 | 7 | 0.13 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG21 | 3 | 0.13 |
| (2,1070) | 2:B:140:ASN:HA | 2:B:143:ILE:HG23 | 3 | 0.13 |
| (1,87) | 2:B:142:VAL:N | 2:B:138:ARG:O | 5 | 0.13 |
| (1,87) | 2:B:142:VAL:N | 2:B:138:ARG:O | 8 | 0.13 |
| (1,82) | 2:B:129:SER:H | 2:B:125:LYS:O | 7 | 0.13 |
| (1,81) | 2:B:129:SER:N | 2:B:125:LYS:O | 7 | 0.13 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 10 | 0.13 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 5 | 0.13 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 6 | 0.13 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 7 | 0.13 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 1 | 0.13 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 4 | 0.13 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 8 | 0.13 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 2 | 0.13 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 8 | 0.13 |
| (1,24) | 1:A:27:LYS:H | 1:A:24:THR:O | 1 | 0.13 |
| (1,19) | 1:A:16:LEU:N | 1:A:12:SER:O | 3 | 0.13 |
| (1,19) | 1:A:16:LEU:N | 1:A:12:SER:O | 9 | 0.13 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 2 | 0.12 |
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 2 | 0.12 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 7 | 0.12 |
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 7 | 0.12 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 9 | 0.12 |
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 9 | 0.12 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 7 | 0.12 |
| (2,850) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 7 | 0.12 |
| (2,850) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 7 | 0.12 |
| (2,850) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 7 | 0.12 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 4 | 0.12 |
| (2,847) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 4 | 0.12 |
| (2,847) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 4 | 0.12 |
| (2,847) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 4 | 0.12 |
| (2,846) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HB2 | 6 | 0.12 |
| (2,846) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB2 | 6 | 0.12 |
| (2,846) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HB3 | 6 | 0.12 |
| (2,846) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HB2 | 6 | 0.12 |
| (2,829) | 2:B:108:LEU:HD12 | 2:B:154:VAL:HB | 3 | 0.12 |
| (2,829) | 2:B:108:LEU:HD13 | 2:B:154:VAL:HB | 3 | 0.12 |
| (2,829) | 2:B:108:LEU:HD12 | 2:B:154:VAL:HB | 8 | 0.12 |
| (2,829) | 2:B:108:LEU:HD13 | 2:B:154:VAL:HB | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG12 | 10 | 0.12 |
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG11 | 10 | 0.12 |
| (2,73) | 1:A:27:LYS:H | 2:B:130:VAL:HG13 | 10 | 0.12 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 8 | 0.12 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 8 | 0.12 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 8 | 0.12 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 8 | 0.12 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 8 | 0.12 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 2 | 0.12 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 2 | 0.12 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 4 | 0.12 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 4 | 0.12 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD13 | 1 | 0.12 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD22 | 1 | 0.12 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD21 | 1 | 0.12 |
| (2,659) | 1:A:46:LEU:H | 1:A:46:LEU:HD23 | 1 | 0.12 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG12 | 3 | 0.12 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG11 | 3 | 0.12 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG13 | 3 | 0.12 |
| (2,61) | 1:A:24:THR:H | 1:A:23:VAL:HG21 | 3 | 0.12 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 4 | 0.12 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 4 | 0.12 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 10 | 0.12 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 10 | 0.12 |
| (2,560) | 1:A:33:LYS:HA | 1:A:33:LYS:HG2 | 5 | 0.12 |
| (2,560) | 1:A:33:LYS:HA | 1:A:33:LYS:HG3 | 5 | 0.12 |
| (2,558) | 1:A:33:LYS:HB2 | 1:A:33:LYS:HD2 | 7 | 0.12 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD2 | 7 | 0.12 |
| (2,558) | 1:A:33:LYS:HB3 | 1:A:33:LYS:HD3 | 7 | 0.12 |
| (2,557) | 1:A:33:LYS:HA | 1:A:33:LYS:HB2 | 8 | 0.12 |
| (2,557) | 1:A:33:LYS:HA | 1:A:33:LYS:HB3 | 8 | 0.12 |
| (2,554) | 1:A:33:LYS:HA | 1:A:33:LYS:HB2 | 8 | 0.12 |
| (2,554) | 1:A:33:LYS:HA | 1:A:33:LYS:HB3 | 8 | 0.12 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 10 | 0.12 |
| (2,4532) | 2:B:151:ILE:HD11 | 2:B:107:TYR:HE1 | 5 | 0.12 |
| (2,4531) | 2:B:151:ILE:HB | 2:B:150:ASN:H | 9 | 0.12 |
| (2,4522) | 2:B:146:LEU:HA | 2:B:146:LEU:HG | 1 | 0.12 |
| (2,4522) | 2:B:146:LEU:HA | 2:B:146:LEU:HG | 6 | 0.12 |
| (2,4514) | 2:B:144:SER:H | 2:B:143:ILE:HA | 2 | 0.12 |
| (2,4514) | 2:B:144:SER:H | 2:B:143:ILE:HA | 5 | 0.12 |
| (2,4512) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 7 | 0.12 |
| (2,4512) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,4512) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 9 | 0.12 |
| (2,4509) | 2:B:142:VAL:HB | 2:B:143:ILE:H | 10 | 0.12 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 2 | 0.12 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 6 | 0.12 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 9 | 0.12 |
| (2,4495) | 2:B:139:LEU:H | 2:B:138:ARG:HA | 10 | 0.12 |
| (2,4446) | 2:B:120:ALA:HA | 2:B:140:ASN:HA | 3 | 0.12 |
| (2,4446) | 2:B:120:ALA:HA | 2:B:140:ASN:HA | 10 | 0.12 |
| (2,4393) | 1:A:63:VAL:HA | 1:A:64:GLY:H | 8 | 0.12 |
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 8 | 0.12 |
| (2,430) | 1:A:15:ILE:HG22 | 2:B:106:SER:HA | 4 | 0.12 |
| (2,430) | 1:A:15:ILE:HG23 | 2:B:106:SER:HA | 4 | 0.12 |
| (2,4251) | 1:A:15:ILE:HA | 2:B:103:TYR:HA | 5 | 0.12 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 5 | 0.12 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 7 | 0.12 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 10 | 0.12 |
| (2,4119) | 2:B:155:ILE:HB | 2:B:152:GLU:HA | 2 | 0.12 |
| (2,4104) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 7 | 0.12 |
| (2,4104) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 8 | 0.12 |
| (2,4104) | 2:B:143:ILE:HA | 2:B:146:LEU:HG | 9 | 0.12 |
| (2,4098) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 8 | 0.12 |
| (2,4098) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 9 | 0.12 |
| (2,4046) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 1 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 1 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 1 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 2 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 2 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 3 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 3 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 4 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 4 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 5 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 5 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 6 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 6 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 7 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 7 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 8 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 8 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 9 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 9 | 0.12 |
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,403) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.12 |
| (2,3954) | 2:B:143:ILE:H | 2:B:107:TYR:HE2 | 1 | 0.12 |
| (2,3954) | 2:B:143:ILE:H | 2:B:107:TYR:HE2 | 5 | 0.12 |
| (2,3954) | 2:B:143:ILE:H | 2:B:107:TYR:HE2 | 8 | 0.12 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB2 | 3 | 0.12 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB3 | 3 | 0.12 |
| (2,3783) | 2:B:108:LEU:H | 2:B:108:LEU:HG | 3 | 0.12 |
| (2,3783) | 2:B:108:LEU:H | 2:B:108:LEU:HG | 10 | 0.12 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 3 | 0.12 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 8 | 0.12 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 10 | 0.12 |
| (2,3728) | 1:A:55:ASN:H | 1:A:54:VAL:H | 4 | 0.12 |
| (2,3668) | 1:A:37:VAL:H | 1:A:37:VAL:HB | 4 | 0.12 |
| (2,3668) | 1:A:37:VAL:H | 1:A:37:VAL:HB | 5 | 0.12 |
| (2,3668) | 1:A:37:VAL:H | 1:A:37:VAL:HB | 8 | 0.12 |
| (2,3668) | 1:A:37:VAL:H | 1:A:37:VAL:HB | 9 | 0.12 |
| (2,3668) | 1:A:37:VAL:H | 1:A:37:VAL:HB | 10 | 0.12 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 2 | 0.12 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 8 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG12 | 7 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG13 | 7 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG23 | 1:A:10:ILE:HG13 | 7 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG12 | 7 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG13 | 7 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG12 | 10 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG21 | 1:A:10:ILE:HG13 | 10 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG23 | 1:A:10:ILE:HG13 | 10 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG12 | 10 | 0.12 |
| (2,3509) | 2:B:159:ILE:HG22 | 1:A:10:ILE:HG13 | 10 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG22 | 6 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG21 | 6 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB2 | 1:A:4:VAL:HG23 | 6 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB3 | 1:A:4:VAL:HG21 | 6 | 0.12 |
| (2,3488) | 2:B:152:GLU:HB3 | 1:A:4:VAL:HG23 | 6 | 0.12 |
| (2,3430) | 1:A:11:TYR:HE1 | 2:B:108:LEU:HD21 | 10 | 0.12 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD21 | 10 | 0.12 |
| (2,3430) | 1:A:11:TYR:HE2 | 2:B:108:LEU:HD23 | 10 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 10 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 10 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 10 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 10 | 0.12 |
| (2,3391) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,337) | 2:B:169:GLY:H | 2:B:168:GLY:HA2 | 4 | 0.12 |
| (2,337) | 2:B:169:GLY:H | 2:B:168:GLY:HA3 | 4 | 0.12 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 4 | 0.12 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 4 | 0.12 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 4 | 0.12 |
| (2,3351) | 1:A:16:LEU:HD12 | 2:B:130:VAL:HA | 8 | 0.12 |
| (2,3351) | 1:A:16:LEU:HD11 | 2:B:130:VAL:HA | 8 | 0.12 |
| (2,3351) | 1:A:16:LEU:HD13 | 2:B:130:VAL:HA | 8 | 0.12 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB2 | 6 | 0.12 |
| (2,335) | 2:B:167:ALA:H | 2:B:166:PRO:HB3 | 6 | 0.12 |
| (2,3331) | 1:A:14:LEU:HD13 | 2:B:159:ILE:HA | 1 | 0.12 |
| (2,3331) | 1:A:14:LEU:HD22 | 2:B:159:ILE:HA | 1 | 0.12 |
| (2,3331) | 1:A:14:LEU:HD21 | 2:B:159:ILE:HA | 1 | 0.12 |
| (2,3331) | 1:A:14:LEU:HD23 | 2:B:159:ILE:HA | 1 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 8 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 8 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 8 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 8 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 8 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 8 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG22 | 9 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG21 | 9 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD12 | 2:B:159:ILE:HG23 | 9 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD11 | 2:B:159:ILE:HG22 | 9 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG22 | 9 | 0.12 |
| (2,3322) | 1:A:10:ILE:HD13 | 2:B:159:ILE:HG21 | 9 | 0.12 |
| (2,3298) | 1:A:1:MET:HG2 | 2:B:153:ASP:HB3 | 6 | 0.12 |
| (2,3298) | 1:A:1:MET:HG3 | 2:B:153:ASP:HB2 | 6 | 0.12 |
| (2,3298) | 1:A:1:MET:HG3 | 2:B:153:ASP:HB3 | 6 | 0.12 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD12 | 8 | 0.12 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD11 | 8 | 0.12 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD13 | 8 | 0.12 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG2 | 1 | 0.12 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG3 | 1 | 0.12 |
| (2,3221) | 2:B:159:ILE:HD12 | 2:B:158:GLY:H | 3 | 0.12 |
| (2,3221) | 2:B:159:ILE:HD13 | 2:B:158:GLY:H | 3 | 0.12 |
| (2,3221) | 2:B:159:ILE:HD12 | 1:A:61:CYS:H | 3 | 0.12 |
| (2,3221) | 2:B:159:ILE:HD13 | 1:A:61:CYS:H | 3 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 9 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 9 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 9 | 0.12 |
| (2,3172) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 9 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3172) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 9 | 0.12 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD23 | 3 | 0.12 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD12 | 3 | 0.12 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD22 | 3 | 0.12 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD21 | 3 | 0.12 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 1 | 0.12 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 1 | 0.12 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 1 | 0.12 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 1 | 0.12 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 1 | 0.12 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 1 | 0.12 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 1 | 0.12 |
| (2,308) | 2:B:150:ASN:H | 2:B:154:VAL:H | 6 | 0.12 |
| (2,308) | 2:B:150:ASN:H | 2:B:153:ASP:H | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG12 | 2:B:107:TYR:HD2 | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG11 | 2:B:107:TYR:HD2 | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG13 | 2:B:107:TYR:HD2 | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD1 | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD2 | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HE2 | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG21 | 2:B:107:TYR:HD2 | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG23 | 2:B:107:TYR:HD2 | 6 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG12 | 2:B:107:TYR:HD2 | 10 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG11 | 2:B:107:TYR:HD2 | 10 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG13 | 2:B:107:TYR:HD2 | 10 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD1 | 10 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HD2 | 10 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG22 | 2:B:107:TYR:HE2 | 10 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG21 | 2:B:107:TYR:HD2 | 10 | 0.12 |
| (2,3054) | 2:B:142:VAL:HG23 | 2:B:107:TYR:HD2 | 10 | 0.12 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD12 | 7 | 0.12 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD11 | 7 | 0.12 |
| (2,3032) | 2:B:140:ASN:HA | 2:B:143:ILE:HD13 | 7 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 1 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 1 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 1 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 2 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 2 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 2 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 4 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 4 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 5 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 5 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 5 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 6 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 6 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 6 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 7 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 7 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 7 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD12 | 2:B:138:ARG:H | 10 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD11 | 2:B:138:ARG:H | 10 | 0.12 |
| (2,3018) | 2:B:139:LEU:HD13 | 2:B:138:ARG:H | 10 | 0.12 |
| (2,3011) | 2:B:137:ASP:HB3 | 2:B:138:ARG:HG2 | 5 | 0.12 |
| (2,3011) | 2:B:137:ASP:HB2 | 2:B:138:ARG:HG2 | 5 | 0.12 |
| (2,3010) | 2:B:138:ARG:HG2 | 2:B:135:ASP:H | 1 | 0.12 |
| (2,3010) | 2:B:138:ARG:HG3 | 2:B:135:ASP:H | 1 | 0.12 |
| (2,2992) | 2:B:137:ASP:HA | 2:B:140:ASN:HB2 | 2 | 0.12 |
| (2,2992) | 2:B:137:ASP:HA | 2:B:140:ASN:HB3 | 2 | 0.12 |
| (2,2982) | 2:B:134:ALA:HB3 | 2:B:124:LYS:HA | 6 | 0.12 |
| (2,2982) | 2:B:134:ALA:HB2 | 2:B:124:LYS:HA | 6 | 0.12 |
| (2,2982) | 2:B:134:ALA:HB1 | 2:B:124:LYS:HA | 6 | 0.12 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB1 | 5 | 0.12 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB3 | 5 | 0.12 |
| (2,2976) | 2:B:134:ALA:HB2 | 2:B:135:ASP:HB3 | 9 | 0.12 |
| (2,2976) | 2:B:134:ALA:HB1 | 2:B:135:ASP:HB3 | 9 | 0.12 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB2 | 9 | 0.12 |
| (2,2976) | 2:B:134:ALA:HB3 | 2:B:135:ASP:HB3 | 9 | 0.12 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG22 | 6 | 0.12 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG21 | 6 | 0.12 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG23 | 6 | 0.12 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG12 | 7 | 0.12 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG11 | 7 | 0.12 |
| (2,287) | 2:B:141:LYS:H | 2:B:142:VAL:HG13 | 7 | 0.12 |
| (2,2861) | 2:B:124:LYS:HE3 | 2:B:124:LYS:HB2 | 4 | 0.12 |
| (2,2861) | 2:B:124:LYS:HE3 | 2:B:124:LYS:HB3 | 4 | 0.12 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE3 | 3 | 0.12 |
| (2,2826) | 2:B:121:LYS:HD2 | 2:B:121:LYS:HE2 | 3 | 0.12 |
| (2,2826) | 2:B:121:LYS:HD3 | 2:B:121:LYS:HE2 | 3 | 0.12 |
| (2,282) | 2:B:140:ASN:H | 2:B:141:LYS:HB2 | 7 | 0.12 |
| (2,282) | 2:B:140:ASN:H | 2:B:141:LYS:HB3 | 7 | 0.12 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 5 | 0.12 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 5 | 0.12 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 6 | 0.12 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 6 | 0.12 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 6 | 0.12 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 9 | 0.12 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 9 | 0.12 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 9 | 0.12 |
| (2,2776) | 2:B:117:SER:HB3 | 2:B:118:PRO:HD3 | 10 | 0.12 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD2 | 10 | 0.12 |
| (2,2776) | 2:B:117:SER:HB2 | 2:B:118:PRO:HD3 | 10 | 0.12 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 1 | 0.12 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 1 | 0.12 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB2 | 3 | 0.12 |
| (2,2759) | 2:B:116:SER:H | 2:B:115:ASN:HB3 | 3 | 0.12 |
| (2,2746) | 2:B:112:LEU:HD22 | 1:A:7:LEU:HG | 8 | 0.12 |
| (2,2746) | 2:B:112:LEU:HD21 | 1:A:7:LEU:HG | 8 | 0.12 |
| (2,2746) | 2:B:112:LEU:HD23 | 1:A:7:LEU:HG | 8 | 0.12 |
| (2,2746) | 2:B:112:LEU:HD11 | 1:A:7:LEU:HG | 8 | 0.12 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB2 | 4 | 0.12 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB1 | 4 | 0.12 |
| (2,2732) | 2:B:117:SER:H | 2:B:111:ALA:HB3 | 4 | 0.12 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 3 | 0.12 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 3 | 0.12 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 3 | 0.12 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 3 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 1 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 1 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 1 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 2 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 2 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 2 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 4 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 4 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 4 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 7 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 7 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 7 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 9 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 9 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 9 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 10 | 0.12 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 10 | 0.12 |
| (2,2717) | 2:B:110:ALA:HB2 | 2:B:115:ASN:HD21 | 3 | 0.12 |
| (2,2717) | 2:B:110:ALA:HB1 | 2:B:115:ASN:HD21 | 3 | 0.12 |
| (2,2717) | 2:B:110:ALA:HB3 | 2:B:115:ASN:HD21 | 3 | 0.12 |
| (2,2716) | 2:B:110:ALA:HB2 | 2:B:118:PRO:HA | 8 | 0.12 |
| (2,2716) | 2:B:110:ALA:HB2 | 2:B:111:ALA:HA | 8 | 0.12 |
| (2,2716) | 2:B:110:ALA:HB1 | 2:B:118:PRO:HA | 8 | 0.12 |
| (2,2716) | 2:B:110:ALA:HB3 | 2:B:118:PRO:HA | 8 | 0.12 |
| (2,264) | 2:B:133:GLU:H | 2:B:134:ALA:HB2 | 4 | 0.12 |
| (2,264) | 2:B:133:GLU:H | 2:B:134:ALA:HB1 | 4 | 0.12 |
| (2,2589) | 1:A:62:ASN:HB3 | 1:A:43:TRP:HZ2 | 10 | 0.12 |
| (2,2589) | 1:A:62:ASN:HB2 | 1:A:43:TRP:HZ2 | 10 | 0.12 |
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 9 | 0.12 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 9 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 4 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 4 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 5 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 5 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 6 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 6 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 10 | 0.12 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 10 | 0.12 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD21 | 2 | 0.12 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD22 | 2 | 0.12 |
| (2,2579) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HD21 | 2 | 0.12 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD21 | 8 | 0.12 |
| (2,2579) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HD22 | 8 | 0.12 |
| (2,2579) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HD21 | 8 | 0.12 |
| (2,2566) | 1:A:60:ILE:HD11 | 1:A:60:ILE:HB | 7 | 0.12 |
| (2,2566) | 1:A:60:ILE:HD13 | 1:A:60:ILE:HB | 7 | 0.12 |
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 9 | 0.12 |
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 9 | 0.12 |
| (2,2527) | 1:A:56:ILE:HD12 | 1:A:17:HIS:HD2 | 2 | 0.12 |
| (2,2527) | 1:A:56:ILE:HD11 | 1:A:17:HIS:HD2 | 2 | 0.12 |
| (2,2527) | 1:A:56:ILE:HD13 | 1:A:17:HIS:HD2 | 2 | 0.12 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD13 | 8 | 0.12 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD12 | 8 | 0.12 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:51:LEU:HD11 | 8 | 0.12 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD11 | 8 | 0.12 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD12 | 8 | 0.12 |
| (2,2462) | 1:A:47:PHE:HB2 | 1:A:59:LEU:HD13 | 8 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 1 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 2 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 2 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 4 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 4 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 5 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 5 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 6 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 6 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 7 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 7 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 8 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 8 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 9 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 9 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 10 | 0.12 |
| (2,2451) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 10 | 0.12 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD2 | 7 | 0.12 |
| (2,244) | 2:B:125:LYS:H | 2:B:125:LYS:HD3 | 7 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG22 | 5 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG21 | 5 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG23 | 5 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG22 | 9 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG21 | 9 | 0.12 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG23 | 9 | 0.12 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 1 | 0.12 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 1 | 0.12 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 8 | 0.12 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 8 | 0.12 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 3 | 0.12 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 3 | 0.12 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 3 | 0.12 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 3 | 0.12 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 3 | 0.12 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 3 | 0.12 |
| (2,2251) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB2 | 2 | 0.12 |
| (2,2251) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB1 | 2 | 0.12 |
| (2,2251) | 1:A:25:GLU:HB2 | 1:A:48:ALA:HB3 | 2 | 0.12 |
| (2,2251) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB1 | 2 | 0.12 |
| (2,2251) | 1:A:25:GLU:HB3 | 1:A:48:ALA:HB3 | 2 | 0.12 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD12 | 2 | 0.12 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD11 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD13 | 2 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG12 | 1:A:51:LEU:H | 3 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG11 | 1:A:51:LEU:H | 3 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG13 | 1:A:51:LEU:H | 3 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG12 | 1:A:51:LEU:H | 9 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG11 | 1:A:51:LEU:H | 9 | 0.12 |
| (2,2238) | 1:A:23:VAL:HG13 | 1:A:51:LEU:H | 9 | 0.12 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 6 | 0.12 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 6 | 0.12 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 6 | 0.12 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 10 | 0.12 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 10 | 0.12 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 10 | 0.12 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE2 | 6 | 0.12 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE1 | 6 | 0.12 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE3 | 6 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 1 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 1 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 2 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 2 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 3 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 3 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 4 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 4 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 5 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 5 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 6 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 6 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 7 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 7 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 8 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 8 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 9 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 9 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.12 |
| (2,2118) | 1:A:11:TYR:HB2 | 1:A:11:TYR:HB3 | 10 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG22 | 1:A:47:PHE:HE2 | 4 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG22 | 1:A:9:CYS:H | 4 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:47:PHE:HE1 | 4 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:47:PHE:HE2 | 4 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:9:CYS:H | 4 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG23 | 1:A:47:PHE:HE1 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2100) | 1:A:10:ILE:HG23 | 1:A:47:PHE:HE2 | 4 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG22 | 1:A:47:PHE:HE2 | 9 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG22 | 1:A:9:CYS:H | 9 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:47:PHE:HE1 | 9 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:47:PHE:HE2 | 9 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG21 | 1:A:9:CYS:H | 9 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG23 | 1:A:47:PHE:HE1 | 9 | 0.12 |
| (2,2100) | 1:A:10:ILE:HG23 | 1:A:47:PHE:HE2 | 9 | 0.12 |
| (2,2072) | 1:A:7:LEU:HD12 | 1:A:7:LEU:H | 1 | 0.12 |
| (2,2072) | 1:A:7:LEU:HD11 | 1:A:7:LEU:H | 1 | 0.12 |
| (2,2072) | 1:A:7:LEU:HD13 | 1:A:7:LEU:H | 1 | 0.12 |
| (2,2072) | 1:A:7:LEU:HD23 | 1:A:7:LEU:H | 1 | 0.12 |
| (2,2050) | 1:A:5:SER:H | 1:A:4:VAL:HG12 | 4 | 0.12 |
| (2,2050) | 1:A:5:SER:H | 1:A:4:VAL:HG11 | 4 | 0.12 |
| (2,2050) | 1:A:5:SER:H | 1:A:4:VAL:HG13 | 4 | 0.12 |
| (2,2050) | 1:A:5:SER:H | 1:A:4:VAL:HG23 | 4 | 0.12 |
| (2,202) | 2:B:114:GLY:H | 2:B:115:ASN:HB3 | 3 | 0.12 |
| (2,202) | 2:B:114:GLY:H | 2:B:115:ASN:HB2 | 3 | 0.12 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 2 | 0.12 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 2 | 0.12 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 2 | 0.12 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 7 | 0.12 |
| (2,1958) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 7 | 0.12 |
| (2,1876) | 2:B:143:ILE:HG21 | 2:B:147:ASN:HB2 | 2 | 0.12 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB2 | 2 | 0.12 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB3 | 2 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG12 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG11 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD12 | 2:B:142:VAL:HG13 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG12 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG11 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD11 | 2:B:142:VAL:HG13 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG12 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG11 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG13 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG22 | 4 | 0.12 |
| (2,1873) | 2:B:143:ILE:HD13 | 2:B:142:VAL:HG23 | 4 | 0.12 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 5 | 0.12 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 5 | 0.12 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE2 | 2 | 0.12 |
| (2,1716) | 2:B:121:LYS:HG2 | 2:B:121:LYS:HE3 | 2 | 0.12 |
| (2,1716) | 2:B:121:LYS:HG3 | 2:B:121:LYS:HE3 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB2 | 3 | 0.12 |
| (2,1701) | 2:B:120:ALA:HB2 | 2:B:139:LEU:HB3 | 3 | 0.12 |
| (2,1701) | 2:B:120:ALA:HB1 | 2:B:139:LEU:HB3 | 3 | 0.12 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB2 | 3 | 0.12 |
| (2,1701) | 2:B:120:ALA:HB3 | 2:B:139:LEU:HB3 | 3 | 0.12 |
| (2,1614) | 2:B:101:MET:HE1 | 1:A:14:LEU:HB2 | 9 | 0.12 |
| (2,1614) | 2:B:101:MET:HE3 | 1:A:14:LEU:HB2 | 9 | 0.12 |
| (2,1614) | 2:B:101:MET:HE2 | 1:A:14:LEU:HB2 | 9 | 0.12 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 1 | 0.12 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 1 | 0.12 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 1 | 0.12 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 1 | 0.12 |
| (2,1561) | 1:A:56:ILE:HD11 | 1:A:10:ILE:HG21 | 2 | 0.12 |
| (2,1561) | 1:A:56:ILE:HD11 | 1:A:10:ILE:HG23 | 2 | 0.12 |
| (2,1561) | 1:A:56:ILE:HD13 | 1:A:10:ILE:HG21 | 2 | 0.12 |
| (2,1561) | 1:A:56:ILE:HD13 | 1:A:10:ILE:HG23 | 2 | 0.12 |
| (2,1561) | 1:A:56:ILE:HD12 | 1:A:10:ILE:HG21 | 2 | 0.12 |
| (2,1561) | 1:A:56:ILE:HD12 | 1:A:10:ILE:HG23 | 2 | 0.12 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 4 | 0.12 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 4 | 0.12 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 4 | 0.12 |
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 8 | 0.12 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 8 | 0.12 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 8 | 0.12 |
| (2,1402) | 1:A:26:ASP:HB2 | 1:A:26:ASP:HA | 6 | 0.12 |
| (2,1402) | 1:A:26:ASP:HB3 | 1:A:26:ASP:HA | 6 | 0.12 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 8 | 0.12 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 8 | 0.12 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 1 | 0.12 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 1 | 0.12 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 1 | 0.12 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 1 | 0.12 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB2 | 9 | 0.12 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB1 | 9 | 0.12 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:13:ALA:HB3 | 9 | 0.12 |
| (2,1329) | 1:A:14:LEU:HA | 1:A:56:ILE:HG23 | 9 | 0.12 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB3 | 1 | 0.12 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB2 | 1 | 0.12 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB3 | 5 | 0.12 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB2 | 5 | 0.12 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB3 | 8 | 0.12 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB2 | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1285) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HB3 | 2 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HB2 | 2 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HB3 | 2 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG12 | 1:A:7:LEU:HB3 | 2 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HB3 | 2 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HB2 | 2 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HB3 | 2 | 0.12 |
| (2,1285) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HB2 | 2 | 0.12 |
| (2,1236) | 2:B:164:SER:HA | 2:B:164:SER:HB2 | 1 | 0.12 |
| (2,1236) | 2:B:164:SER:HA | 2:B:164:SER:HB3 | 1 | 0.12 |
| (2,1216) | 2:B:159:ILE:HG12 | 2:B:159:ILE:HG22 | 5 | 0.12 |
| (2,1216) | 2:B:159:ILE:HG13 | 2:B:159:ILE:HG22 | 5 | 0.12 |
| (2,1216) | 2:B:159:ILE:HG13 | 2:B:159:ILE:HG21 | 5 | 0.12 |
| (2,1216) | 2:B:159:ILE:HG13 | 2:B:159:ILE:HG23 | 5 | 0.12 |
| (2,1191) | 2:B:157:GLN:HB2 | 2:B:154:VAL:HA | 5 | 0.12 |
| (2,1191) | 2:B:157:GLN:HB3 | 2:B:154:VAL:HA | 5 | 0.12 |
| (2,1191) | 2:B:157:GLN:HB2 | 2:B:154:VAL:HA | 8 | 0.12 |
| (2,1191) | 2:B:157:GLN:HB3 | 2:B:154:VAL:HA | 8 | 0.12 |
| (2,1162) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 3 | 0.12 |
| (2,1162) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 3 | 0.12 |
| (2,1162) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 3 | 0.12 |
| (2,1154) | 2:B:151:ILE:HG22 | 2:B:152:GLU:HG2 | 1 | 0.12 |
| (2,1154) | 2:B:151:ILE:HG21 | 2:B:152:GLU:HG2 | 1 | 0.12 |
| (2,1154) | 2:B:151:ILE:HG23 | 2:B:152:GLU:HG2 | 1 | 0.12 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 5 | 0.12 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 5 | 0.12 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 10 | 0.12 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 10 | 0.12 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD11 | 7 | 0.12 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD13 | 7 | 0.12 |
| (2,1132) | 2:B:146:LEU:HD22 | 2:B:142:VAL:HA | 7 | 0.12 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD21 | 7 | 0.12 |
| (2,1132) | 2:B:146:LEU:HD21 | 2:B:142:VAL:HA | 7 | 0.12 |
| (2,1132) | 2:B:143:ILE:HA | 2:B:146:LEU:HD12 | 7 | 0.12 |
| (2,1132) | 2:B:146:LEU:HD12 | 2:B:142:VAL:HA | 7 | 0.12 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB3 | 3 | 0.12 |
| (2,1114) | 2:B:144:SER:HA | 2:B:144:SER:HB2 | 3 | 0.12 |
| (2,1112) | 2:B:143:ILE:HG21 | 2:B:119:SER:HB2 | 5 | 0.12 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB2 | 5 | 0.12 |
| (2,1112) | 2:B:143:ILE:HG23 | 2:B:119:SER:HB3 | 5 | 0.12 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 1 | 0.12 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 1 | 0.12 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 1 | 0.12 |
| (2,1064) | 2:B:137:ASP:HA | 2:B:139:LEU:HD12 | 8 | 0.12 |
| (2,1064) | 2:B:137:ASP:HA | 2:B:139:LEU:HD11 | 8 | 0.12 |
| (2,1064) | 2:B:137:ASP:HA | 2:B:139:LEU:HD13 | 8 | 0.12 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG2 | 9 | 0.12 |
| (2,1051) | 2:B:139:LEU:HA | 2:B:141:LYS:HG3 | 9 | 0.12 |
| (2,1028) | 2:B:134:ALA:HB1 | 2:B:124:LYS:HA | 6 | 0.12 |
| (2,1028) | 2:B:134:ALA:HB3 | 2:B:124:LYS:HA | 6 | 0.12 |
| (2,1028) | 2:B:134:ALA:HB2 | 2:B:124:LYS:HA | 6 | 0.12 |
| (1,99) | 2:B:155:ILE:N | 2:B:151:ILE:O | 1 | 0.12 |
| (1,99) | 2:B:155:ILE:N | 2:B:151:ILE:O | 9 | 0.12 |
| (1,91) | 2:B:144:SER:N | 2:B:140:ASN:O | 5 | 0.12 |
| (1,87) | 2:B:142:VAL:N | 2:B:138:ARG:O | 2 | 0.12 |
| (1,87) | 2:B:142:VAL:N | 2:B:138:ARG:O | 6 | 0.12 |
| (1,87) | 2:B:142:VAL:N | 2:B:138:ARG:O | 7 | 0.12 |
| (1,82) | 2:B:129:SER:H | 2:B:125:LYS:O | 5 | 0.12 |
| (1,81) | 2:B:129:SER:N | 2:B:125:LYS:O | 5 | 0.12 |
| (1,73) | 2:B:125:LYS:N | 2:B:121:LYS:O | 3 | 0.12 |
| (1,61) | 2:B:110:ALA:N | 2:B:106:SER:O | 1 | 0.12 |
| (1,6) | 1:A:9:CYS:H | 1:A:5:SER:O | 6 | 0.12 |
| (1,55) | 2:B:107:TYR:N | 2:B:103:TYR:O | 1 | 0.12 |
| (1,55) | 2:B:107:TYR:N | 2:B:103:TYR:O | 5 | 0.12 |
| (1,55) | 2:B:107:TYR:N | 2:B:103:TYR:O | 9 | 0.12 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 2 | 0.12 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 4 | 0.12 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 1 | 0.12 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 4 | 0.12 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 8 | 0.12 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 2 | 0.12 |
| (1,32) | 1:A:31:LEU:H | 1:A:27:LYS:O | 1 | 0.12 |
| (1,32) | 1:A:31:LEU:H | 1:A:27:LYS:O | 3 | 0.12 |
| (1,13) | 1:A:13:ALA:N | 1:A:9:CYS:O | 4 | 0.12 |
| (1,13) | 1:A:13:ALA:N | 1:A:9:CYS:O | 8 | 0.12 |
| (1,13) | 1:A:13:ALA:N | 1:A:9:CYS:O | 9 | 0.12 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 1 | 0.11 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 1 | 0.11 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 3 | 0.11 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 3 | 0.11 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 5 | 0.11 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 5 | 0.11 |
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB2 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,918) | 2:B:121:LYS:HA | 2:B:121:LYS:HB3 | 6 | 0.11 |
| (2,907) | 2:B:118:PRO:HG3 | 2:B:117:SER:HA | 1 | 0.11 |
| (2,907) | 2:B:118:PRO:HG2 | 2:B:117:SER:HA | 1 | 0.11 |
| (2,881) | 2:B:116:SER:HA | 2:B:116:SER:HB2 | 2 | 0.11 |
| (2,881) | 2:B:116:SER:HA | 2:B:116:SER:HB3 | 2 | 0.11 |
| (2,856) | 2:B:111:ALA:HB1 | 2:B:107:TYR:HE1 | 10 | 0.11 |
| (2,856) | 2:B:111:ALA:HB3 | 2:B:107:TYR:HE1 | 10 | 0.11 |
| (2,856) | 2:B:111:ALA:HB3 | 2:B:107:TYR:HD1 | 10 | 0.11 |
| (2,856) | 2:B:111:ALA:HB2 | 2:B:107:TYR:HE1 | 10 | 0.11 |
| (2,856) | 2:B:111:ALA:HB2 | 2:B:107:TYR:HD1 | 10 | 0.11 |
| (2,829) | 2:B:108:LEU:HD12 | 2:B:154:VAL:HB | 4 | 0.11 |
| (2,829) | 2:B:108:LEU:HD13 | 2:B:154:VAL:HB | 4 | 0.11 |
| (2,829) | 2:B:108:LEU:HD12 | 2:B:154:VAL:HB | 6 | 0.11 |
| (2,829) | 2:B:108:LEU:HD13 | 2:B:154:VAL:HB | 6 | 0.11 |
| (2,829) | 2:B:108:LEU:HD12 | 2:B:154:VAL:HB | 7 | 0.11 |
| (2,829) | 2:B:108:LEU:HD13 | 2:B:154:VAL:HB | 7 | 0.11 |
| (2,739) | 1:A:59:LEU:HD12 | 1:A:56:ILE:HA | 2 | 0.11 |
| (2,739) | 1:A:59:LEU:HD11 | 1:A:56:ILE:HA | 2 | 0.11 |
| (2,739) | 1:A:59:LEU:HD13 | 1:A:56:ILE:HA | 2 | 0.11 |
| (2,739) | 1:A:59:LEU:HD21 | 1:A:56:ILE:HA | 2 | 0.11 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG22 | 5 | 0.11 |
| (2,711) | 1:A:55:ASN:HA | 1:A:56:ILE:HG23 | 5 | 0.11 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG22 | 5 | 0.11 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG21 | 5 | 0.11 |
| (2,711) | 1:A:55:ASN:HA | 1:A:54:VAL:HG23 | 5 | 0.11 |
| (2,695) | 1:A:51:LEU:HD12 | 1:A:48:ALA:HA | 5 | 0.11 |
| (2,695) | 1:A:51:LEU:HD11 | 1:A:48:ALA:HA | 5 | 0.11 |
| (2,695) | 1:A:51:LEU:HD13 | 1:A:48:ALA:HA | 5 | 0.11 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 3 | 0.11 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 3 | 0.11 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 5 | 0.11 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 5 | 0.11 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD2 | 10 | 0.11 |
| (2,678) | 1:A:49:LYS:HA | 1:A:49:LYS:HD3 | 10 | 0.11 |
| (2,673) | 1:A:49:LYS:HB2 | 1:A:49:LYS:HD2 | 6 | 0.11 |
| (2,673) | 1:A:49:LYS:HB3 | 1:A:49:LYS:HD2 | 6 | 0.11 |
| (2,673) | 1:A:49:LYS:HB3 | 1:A:49:LYS:HD3 | 6 | 0.11 |
| (2,66) | 1:A:25:GLU:H | 1:A:24:THR:HG21 | 2 | 0.11 |
| (2,66) | 1:A:25:GLU:H | 1:A:24:THR:HG22 | 2 | 0.11 |
| (2,66) | 1:A:25:GLU:H | 1:A:24:THR:HG23 | 2 | 0.11 |
| (2,650) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 3 | 0.11 |
| (2,650) | 1:A:46:LEU:HB2 | 1:A:46:LEU:HB3 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,617) | 1:A:40:GLU:HG2 | 1:A:40:GLU:HA | 1 | 0.11 |
| (2,617) | 1:A:40:GLU:HG3 | 1:A:40:GLU:HA | 1 | 0.11 |
| (2,617) | 1:A:40:GLU:HG2 | 1:A:40:GLU:HA | 2 | 0.11 |
| (2,617) | 1:A:40:GLU:HG3 | 1:A:40:GLU:HA | 2 | 0.11 |
| (2,617) | 1:A:40:GLU:HG2 | 1:A:40:GLU:HA | 7 | 0.11 |
| (2,617) | 1:A:40:GLU:HG3 | 1:A:40:GLU:HA | 7 | 0.11 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 1 | 0.11 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 1 | 0.11 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 6 | 0.11 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 6 | 0.11 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 7 | 0.11 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 7 | 0.11 |
| (2,6) | 1:A:59:LEU:H | 1:A:55:ASN:O | 9 | 0.11 |
| (2,6) | 1:A:59:LEU:H | 1:A:56:ILE:O | 9 | 0.11 |
| (2,594) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 10 | 0.11 |
| (2,594) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 10 | 0.11 |
| (2,594) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 10 | 0.11 |
| (2,594) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 10 | 0.11 |
| (2,594) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 10 | 0.11 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG22 | 3 | 0.11 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG21 | 3 | 0.11 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG23 | 3 | 0.11 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG22 | 4 | 0.11 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG21 | 4 | 0.11 |
| (2,467) | 1:A:22:THR:HA | 1:A:23:VAL:HG23 | 4 | 0.11 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD12 | 5 | 0.11 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD11 | 5 | 0.11 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD13 | 5 | 0.11 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD22 | 5 | 0.11 |
| (2,46) | 1:A:17:HIS:H | 1:A:16:LEU:HD21 | 5 | 0.11 |
| (2,4570) | 1:A:14:LEU:HG | 2:B:159:ILE:HA | 3 | 0.11 |
| (2,4561) | 2:B:162:LEU:HG | 2:B:162:LEU:H | 1 | 0.11 |
| (2,455) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG22 | 8 | 0.11 |
| (2,455) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG21 | 8 | 0.11 |
| (2,455) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG23 | 8 | 0.11 |
| (2,455) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HD12 | 8 | 0.11 |
| (2,455) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HG21 | 8 | 0.11 |
| (2,455) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HG23 | 8 | 0.11 |
| (2,455) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HD12 | 8 | 0.11 |
| (2,4522) | 2:B:146:LEU:HA | 2:B:146:LEU:HG | 3 | 0.11 |
| (2,4522) | 2:B:146:LEU:HA | 2:B:146:LEU:HG | 4 | 0.11 |
| (2,4514) | 2:B:144:SER:H | 2:B:143:ILE:HA | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,4514) | 2:B:144:SER:H | 2:B:143:ILE:HA | 4 | 0.11 |
| (2,4514) | 2:B:144:SER:H | 2:B:143:ILE:HA | 7 | 0.11 |
| (2,4514) | 2:B:144:SER:H | 2:B:143:ILE:HA | 8 | 0.11 |
| (2,4514) | 2:B:144:SER:H | 2:B:143:ILE:HA | 10 | 0.11 |
| (2,4503) | 2:B:140:ASN:HA | 2:B:141:LYS:H | 4 | 0.11 |
| (2,4503) | 2:B:140:ASN:HA | 2:B:141:LYS:H | 6 | 0.11 |
| (2,4503) | 2:B:140:ASN:HA | 2:B:141:LYS:H | 8 | 0.11 |
| (2,4503) | 2:B:140:ASN:HA | 2:B:141:LYS:H | 10 | 0.11 |
| (2,4393) | 1:A:63:VAL:HA | 1:A:64:GLY:H | 6 | 0.11 |
| (2,4393) | 1:A:63:VAL:HA | 1:A:64:GLY:H | 7 | 0.11 |
| (2,4345) | 1:A:43:TRP:HA | 1:A:46:LEU:HG | 7 | 0.11 |
| (2,4341) | 1:A:41:PRO:HA | 1:A:39:VAL:H | 1 | 0.11 |
| (2,4341) | 1:A:41:PRO:HA | 1:A:39:VAL:H | 10 | 0.11 |
| (2,430) | 1:A:15:ILE:HG22 | 2:B:106:SER:HA | 6 | 0.11 |
| (2,430) | 1:A:15:ILE:HG23 | 2:B:106:SER:HA | 6 | 0.11 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD12 | 3 | 0.11 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD11 | 3 | 0.11 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD13 | 3 | 0.11 |
| (2,43) | 1:A:16:LEU:H | 1:A:16:LEU:HD21 | 3 | 0.11 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 3 | 0.11 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 6 | 0.11 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 8 | 0.11 |
| (2,4250) | 1:A:14:LEU:HG | 1:A:11:TYR:HA | 9 | 0.11 |
| (2,4212) | 1:A:3:SER:HA | 1:A:4:VAL:HB | 3 | 0.11 |
| (2,4173) | 2:B:105:ALA:HA | 2:B:108:LEU:HD22 | 3 | 0.11 |
| (2,4150) | 1:A:39:VAL:HB | 1:A:5:SER:HA | 9 | 0.11 |
| (2,4136) | 1:A:22:THR:HA | 1:A:22:THR:HB | 7 | 0.11 |
| (2,4136) | 1:A:22:THR:HA | 1:A:22:THR:HB | 10 | 0.11 |
| (2,4098) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 3 | 0.11 |
| (2,4098) | 2:B:138:ARG:HA | 2:B:138:ARG:HG2 | 5 | 0.11 |
| (2,4046) | 1:A:56:ILE:HG12 | 1:A:56:ILE:HA | 8 | 0.11 |
| (2,4039) | 1:A:46:LEU:HA | 1:A:46:LEU:HB3 | 3 | 0.11 |
| (2,4017) | 1:A:15:ILE:HA | 2:B:132:ILE:HB | 9 | 0.11 |
| (2,4) | 1:A:37:VAL:H | 1:A:33:LYS:O | 3 | 0.11 |
| (2,4) | 1:A:37:VAL:H | 1:A:32:ILE:O | 3 | 0.11 |
| (2,3838) | 2:B:122:ASP:H | 2:B:120:ALA:H | 9 | 0.11 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB2 | 4 | 0.11 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB3 | 4 | 0.11 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB2 | 7 | 0.11 |
| (2,38) | 1:A:13:ALA:H | 1:A:12:SER:HB3 | 7 | 0.11 |
| (2,3783) | 2:B:108:LEU:H | 2:B:108:LEU:HG | 4 | 0.11 |
| (2,3755) | 1:A:65:ALA:H | 1:A:66:GLY:H | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3745) | 1:A:61:CYS:H | 1:A:62:ASN:HA | 6 | 0.11 |
| (2,3745) | 1:A:61:CYS:H | 1:A:62:ASN:HA | 9 | 0.11 |
| (2,3736) | 1:A:58:SER:H | 1:A:55:ASN:HA | 1 | 0.11 |
| (2,3736) | 1:A:58:SER:H | 1:A:55:ASN:HA | 7 | 0.11 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 5 | 0.11 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 6 | 0.11 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 7 | 0.11 |
| (2,3731) | 1:A:57:GLY:H | 1:A:58:SER:HA | 9 | 0.11 |
| (2,3728) | 1:A:55:ASN:H | 1:A:54:VAL:H | 1 | 0.11 |
| (2,3668) | 1:A:37:VAL:H | 1:A:37:VAL:HB | 2 | 0.11 |
| (2,3668) | 1:A:37:VAL:H | 1:A:37:VAL:HB | 6 | 0.11 |
| (2,3565) | 1:A:14:LEU:H | 1:A:14:LEU:HB3 | 3 | 0.11 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 7 | 0.11 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 9 | 0.11 |
| (2,3541) | 1:A:9:CYS:H | 1:A:10:ILE:HB | 10 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD13 | 1 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD12 | 1 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD11 | 1 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD12 | 1:A:59:LEU:HD13 | 1 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD12 | 1 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD11 | 1 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD11 | 1:A:59:LEU:HD13 | 1 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD12 | 1 | 0.11 |
| (2,3500) | 2:B:159:ILE:HD13 | 1:A:59:LEU:HD11 | 1 | 0.11 |
| (2,3391) | 1:A:37:VAL:HG11 | 2:B:112:LEU:HB3 | 5 | 0.11 |
| (2,3391) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HB3 | 5 | 0.11 |
| (2,3391) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HB3 | 5 | 0.11 |
| (2,3391) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HB3 | 5 | 0.11 |
| (2,3391) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HB3 | 5 | 0.11 |
| (2,337) | 2:B:169:GLY:H | 2:B:168:GLY:HA2 | 10 | 0.11 |
| (2,337) | 2:B:169:GLY:H | 2:B:168:GLY:HA3 | 10 | 0.11 |
| (2,3354) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG22 | 8 | 0.11 |
| (2,3354) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG21 | 8 | 0.11 |
| (2,3354) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG23 | 8 | 0.11 |
| (2,3354) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HD12 | 8 | 0.11 |
| (2,3354) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HG21 | 8 | 0.11 |
| (2,3354) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HG23 | 8 | 0.11 |
| (2,3354) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HD12 | 8 | 0.11 |
| (2,3347) | 1:A:15:ILE:HG22 | 2:B:101:MET:HE2 | 8 | 0.11 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE2 | 8 | 0.11 |
| (2,3347) | 1:A:15:ILE:HG21 | 2:B:101:MET:HE3 | 8 | 0.11 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE2 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE1 | 8 | 0.11 |
| (2,3347) | 1:A:15:ILE:HG23 | 2:B:101:MET:HE3 | 8 | 0.11 |
| (2,3331) | 1:A:14:LEU:HD13 | 2:B:159:ILE:HA | 4 | 0.11 |
| (2,3331) | 1:A:14:LEU:HD22 | 2:B:159:ILE:HA | 4 | 0.11 |
| (2,3331) | 1:A:14:LEU:HD21 | 2:B:159:ILE:HA | 4 | 0.11 |
| (2,3331) | 1:A:14:LEU:HD23 | 2:B:159:ILE:HA | 4 | 0.11 |
| (2,3301) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HA | 4 | 0.11 |
| (2,3301) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HA | 4 | 0.11 |
| (2,3301) | 1:A:2:ALA:HB3 | 2:B:152:GLU:HA | 8 | 0.11 |
| (2,3301) | 1:A:2:ALA:HB1 | 2:B:152:GLU:HA | 8 | 0.11 |
| (2,3270) | 2:B:165:VAL:HG12 | 2:B:161:LYS:HG2 | 7 | 0.11 |
| (2,3270) | 2:B:165:VAL:HG12 | 2:B:161:LYS:HG3 | 7 | 0.11 |
| (2,3270) | 2:B:165:VAL:HG11 | 2:B:161:LYS:HG2 | 7 | 0.11 |
| (2,3270) | 2:B:165:VAL:HG11 | 2:B:161:LYS:HG3 | 7 | 0.11 |
| (2,3270) | 2:B:165:VAL:HG13 | 2:B:161:LYS:HG3 | 7 | 0.11 |
| (2,3270) | 2:B:165:VAL:HG23 | 2:B:161:LYS:HG2 | 7 | 0.11 |
| (2,3270) | 2:B:165:VAL:HG23 | 2:B:161:LYS:HG3 | 7 | 0.11 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD12 | 6 | 0.11 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD11 | 6 | 0.11 |
| (2,3251) | 2:B:162:LEU:HA | 2:B:162:LEU:HD13 | 6 | 0.11 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG2 | 8 | 0.11 |
| (2,324) | 2:B:161:LYS:H | 2:B:161:LYS:HG3 | 8 | 0.11 |
| (2,3239) | 2:B:161:LYS:HD2 | 2:B:161:LYS:HA | 2 | 0.11 |
| (2,3239) | 2:B:161:LYS:HD3 | 2:B:161:LYS:HA | 2 | 0.11 |
| (2,3235) | 2:B:159:ILE:HG13 | 2:B:159:ILE:HG23 | 5 | 0.11 |
| (2,3235) | 2:B:159:ILE:HG12 | 2:B:159:ILE:HG22 | 5 | 0.11 |
| (2,3235) | 2:B:159:ILE:HG13 | 2:B:159:ILE:HG22 | 5 | 0.11 |
| (2,3235) | 2:B:159:ILE:HG13 | 2:B:159:ILE:HG21 | 5 | 0.11 |
| (2,3205) | 2:B:156:ALA:HB2 | 2:B:157:GLN:HG2 | 2 | 0.11 |
| (2,3205) | 2:B:156:ALA:HB1 | 2:B:157:GLN:HG2 | 2 | 0.11 |
| (2,3205) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG2 | 2 | 0.11 |
| (2,3205) | 2:B:156:ALA:HB3 | 2:B:157:GLN:HG3 | 2 | 0.11 |
| (2,3172) | 2:B:154:VAL:HG12 | 2:B:155:ILE:H | 3 | 0.11 |
| (2,3172) | 2:B:154:VAL:HG11 | 2:B:155:ILE:H | 3 | 0.11 |
| (2,3172) | 2:B:154:VAL:HG13 | 2:B:155:ILE:H | 3 | 0.11 |
| (2,3172) | 2:B:154:VAL:HG21 | 2:B:155:ILE:H | 3 | 0.11 |
| (2,3172) | 2:B:154:VAL:HG23 | 2:B:155:ILE:H | 3 | 0.11 |
| (2,3162) | 2:B:154:VAL:HG12 | 2:B:154:VAL:HA | 9 | 0.11 |
| (2,3162) | 2:B:154:VAL:HG13 | 2:B:154:VAL:HA | 9 | 0.11 |
| (2,3162) | 2:B:154:VAL:HG22 | 2:B:154:VAL:HA | 9 | 0.11 |
| (2,3162) | 2:B:154:VAL:HG21 | 2:B:154:VAL:HA | 9 | 0.11 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD23 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD12 | 8 | 0.11 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD22 | 8 | 0.11 |
| (2,31) | 1:A:12:SER:H | 2:B:109:LEU:HD21 | 8 | 0.11 |
| (2,3099) | 2:B:146:LEU:HD23 | 2:B:149:LYS:HE3 | 9 | 0.11 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE2 | 9 | 0.11 |
| (2,3099) | 2:B:146:LEU:HD12 | 2:B:149:LYS:HE3 | 9 | 0.11 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE2 | 9 | 0.11 |
| (2,3099) | 2:B:146:LEU:HD11 | 2:B:149:LYS:HE3 | 9 | 0.11 |
| (2,3099) | 2:B:146:LEU:HD13 | 2:B:149:LYS:HE3 | 9 | 0.11 |
| (2,3099) | 2:B:146:LEU:HD22 | 2:B:149:LYS:HE3 | 9 | 0.11 |
| (2,3074) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD13 | 3 | 0.11 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD12 | 3 | 0.11 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD11 | 3 | 0.11 |
| (2,3074) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD13 | 3 | 0.11 |
| (2,3074) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD12 | 3 | 0.11 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 9 | 0.11 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 9 | 0.11 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 9 | 0.11 |
| (2,3055) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 9 | 0.11 |
| (2,3025) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HE2 | 8 | 0.11 |
| (2,3025) | 2:B:139:LEU:HD21 | 2:B:124:LYS:HE3 | 8 | 0.11 |
| (2,3025) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HE2 | 8 | 0.11 |
| (2,3025) | 2:B:139:LEU:HD23 | 2:B:124:LYS:HE3 | 8 | 0.11 |
| (2,3025) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HE2 | 8 | 0.11 |
| (2,3025) | 2:B:139:LEU:HD22 | 2:B:124:LYS:HE3 | 8 | 0.11 |
| (2,3011) | 2:B:137:ASP:HB3 | 2:B:138:ARG:HG2 | 4 | 0.11 |
| (2,3011) | 2:B:137:ASP:HB2 | 2:B:138:ARG:HG2 | 4 | 0.11 |
| (2,2992) | 2:B:137:ASP:HA | 2:B:140:ASN:HB2 | 9 | 0.11 |
| (2,2992) | 2:B:137:ASP:HA | 2:B:140:ASN:HB3 | 9 | 0.11 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB1 | 1 | 0.11 |
| (2,2981) | 2:B:134:ALA:H | 2:B:134:ALA:HB3 | 1 | 0.11 |
| (2,296) | 2:B:144:SER:H | 2:B:141:LYS:HG2 | 3 | 0.11 |
| (2,296) | 2:B:144:SER:H | 2:B:141:LYS:HG3 | 3 | 0.11 |
| (2,296) | 2:B:144:SER:H | 2:B:141:LYS:HG2 | 6 | 0.11 |
| (2,296) | 2:B:144:SER:H | 2:B:141:LYS:HG3 | 6 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG22 | 2 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG21 | 2 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG23 | 2 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG22 | 5 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG21 | 5 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG23 | 5 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG22 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG21 | 7 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG23 | 7 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG22 | 8 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG21 | 8 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG23 | 8 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG22 | 9 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG21 | 9 | 0.11 |
| (2,291) | 2:B:143:ILE:H | 2:B:143:ILE:HG23 | 9 | 0.11 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB3 | 6 | 0.11 |
| (2,28) | 1:A:11:TYR:H | 1:A:9:CYS:HB2 | 6 | 0.11 |
| (2,2722) | 2:B:110:ALA:HB1 | 2:B:109:LEU:HB3 | 2 | 0.11 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB2 | 2 | 0.11 |
| (2,2722) | 2:B:110:ALA:HB3 | 2:B:109:LEU:HB3 | 2 | 0.11 |
| (2,2722) | 2:B:110:ALA:HB2 | 2:B:109:LEU:HB3 | 2 | 0.11 |
| (2,2721) | 2:B:110:ALA:HB2 | 2:B:119:SER:H | 3 | 0.11 |
| (2,2721) | 2:B:110:ALA:HB1 | 2:B:119:SER:H | 3 | 0.11 |
| (2,2721) | 2:B:110:ALA:HB3 | 2:B:119:SER:H | 3 | 0.11 |
| (2,2703) | 2:B:109:LEU:HD12 | 2:B:109:LEU:H | 1 | 0.11 |
| (2,2703) | 2:B:109:LEU:HD13 | 2:B:109:LEU:H | 1 | 0.11 |
| (2,2703) | 2:B:109:LEU:HD22 | 2:B:109:LEU:H | 1 | 0.11 |
| (2,2703) | 2:B:109:LEU:HD21 | 2:B:109:LEU:H | 1 | 0.11 |
| (2,2703) | 2:B:109:LEU:HD12 | 2:B:109:LEU:H | 3 | 0.11 |
| (2,2703) | 2:B:109:LEU:HD13 | 2:B:109:LEU:H | 3 | 0.11 |
| (2,2703) | 2:B:109:LEU:HD22 | 2:B:109:LEU:H | 3 | 0.11 |
| (2,2703) | 2:B:109:LEU:HD21 | 2:B:109:LEU:H | 3 | 0.11 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:102:ARG:H | 8 | 0.11 |
| (2,2627) | 2:B:101:MET:HE2 | 2:B:103:TYR:H | 8 | 0.11 |
| (2,2627) | 2:B:101:MET:HE1 | 2:B:102:ARG:H | 8 | 0.11 |
| (2,2627) | 2:B:101:MET:HE3 | 2:B:104:VAL:H | 8 | 0.11 |
| (2,2607) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD2 | 10 | 0.11 |
| (2,2607) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD2 | 10 | 0.11 |
| (2,2607) | 1:A:51:LEU:HD12 | 1:A:47:PHE:HD1 | 10 | 0.11 |
| (2,2607) | 1:A:51:LEU:HD11 | 1:A:47:PHE:HD1 | 10 | 0.11 |
| (2,2607) | 1:A:51:LEU:HD13 | 1:A:47:PHE:HD1 | 10 | 0.11 |
| (2,2607) | 1:A:59:LEU:HD13 | 1:A:47:PHE:HD1 | 10 | 0.11 |
| (2,2607) | 1:A:59:LEU:HD23 | 1:A:47:PHE:HD2 | 10 | 0.11 |
| (2,2607) | 1:A:59:LEU:HD13 | 1:A:47:PHE:HD2 | 10 | 0.11 |
| (2,2607) | 1:A:59:LEU:HD23 | 1:A:47:PHE:HD1 | 10 | 0.11 |
| (2,2589) | 1:A:62:ASN:HB3 | 1:A:43:TRP:HZ2 | 3 | 0.11 |
| (2,2589) | 1:A:62:ASN:HB2 | 1:A:43:TRP:HZ2 | 3 | 0.11 |
| (2,2589) | 1:A:62:ASN:HB3 | 1:A:43:TRP:HZ2 | 8 | 0.11 |
| (2,2589) | 1:A:62:ASN:HB2 | 1:A:43:TRP:HZ2 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2584) | 1:A:61:CYS:HB2 | 1:A:62:ASN:HA | 8 | 0.11 |
| (2,2584) | 1:A:61:CYS:HB3 | 1:A:62:ASN:HA | 8 | 0.11 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 3 | 0.11 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 3 | 0.11 |
| (2,2581) | 1:A:61:CYS:HB3 | 1:A:60:ILE:H | 9 | 0.11 |
| (2,2581) | 1:A:61:CYS:HB2 | 1:A:60:ILE:H | 9 | 0.11 |
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 6 | 0.11 |
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 6 | 0.11 |
| (2,2543) | 1:A:58:SER:HB2 | 1:A:59:LEU:HG | 8 | 0.11 |
| (2,2543) | 1:A:58:SER:HB3 | 1:A:59:LEU:HG | 8 | 0.11 |
| (2,2456) | 1:A:46:LEU:HD22 | 1:A:42:PHE:HZ | 4 | 0.11 |
| (2,2456) | 1:A:46:LEU:HD21 | 1:A:42:PHE:HZ | 4 | 0.11 |
| (2,2456) | 1:A:46:LEU:HD23 | 1:A:42:PHE:HZ | 4 | 0.11 |
| (2,2456) | 1:A:46:LEU:HD22 | 1:A:42:PHE:HZ | 6 | 0.11 |
| (2,2456) | 1:A:46:LEU:HD21 | 1:A:42:PHE:HZ | 6 | 0.11 |
| (2,2456) | 1:A:46:LEU:HD23 | 1:A:42:PHE:HZ | 6 | 0.11 |
| (2,2417) | 1:A:40:GLU:HG2 | 1:A:40:GLU:HA | 1 | 0.11 |
| (2,2417) | 1:A:40:GLU:HG3 | 1:A:40:GLU:HA | 1 | 0.11 |
| (2,2417) | 1:A:40:GLU:HG2 | 1:A:40:GLU:HA | 2 | 0.11 |
| (2,2417) | 1:A:40:GLU:HG3 | 1:A:40:GLU:HA | 2 | 0.11 |
| (2,2417) | 1:A:40:GLU:HG2 | 1:A:40:GLU:HA | 7 | 0.11 |
| (2,2417) | 1:A:40:GLU:HG3 | 1:A:40:GLU:HA | 7 | 0.11 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG22 | 4 | 0.11 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG21 | 4 | 0.11 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG23 | 4 | 0.11 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG22 | 10 | 0.11 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG21 | 10 | 0.11 |
| (2,2396) | 1:A:39:VAL:H | 1:A:39:VAL:HG23 | 10 | 0.11 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB2 | 2 | 0.11 |
| (2,2384) | 1:A:37:VAL:HA | 1:A:38:ASN:HB3 | 2 | 0.11 |
| (2,2372) | 1:A:37:VAL:HG21 | 2:B:112:LEU:HG | 6 | 0.11 |
| (2,2372) | 1:A:37:VAL:HG23 | 1:A:4:VAL:HB | 6 | 0.11 |
| (2,2372) | 1:A:37:VAL:HG23 | 2:B:112:LEU:HG | 6 | 0.11 |
| (2,2372) | 1:A:37:VAL:HG13 | 2:B:112:LEU:HG | 6 | 0.11 |
| (2,2372) | 1:A:37:VAL:HG22 | 1:A:4:VAL:HB | 6 | 0.11 |
| (2,2372) | 1:A:37:VAL:HG22 | 2:B:112:LEU:HG | 6 | 0.11 |
| (2,2370) | 1:A:38:ASN:H | 1:A:37:VAL:HG22 | 5 | 0.11 |
| (2,2370) | 1:A:38:ASN:H | 1:A:37:VAL:HG21 | 5 | 0.11 |
| (2,2370) | 1:A:38:ASN:H | 1:A:37:VAL:HG23 | 5 | 0.11 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD12 | 5 | 0.11 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD11 | 5 | 0.11 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD13 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD12 | 8 | 0.11 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD11 | 8 | 0.11 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD13 | 8 | 0.11 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD12 | 9 | 0.11 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD11 | 9 | 0.11 |
| (2,225) | 2:B:120:ALA:H | 2:B:143:ILE:HD13 | 9 | 0.11 |
| (2,2238) | 1:A:23:VAL:HG12 | 1:A:51:LEU:H | 10 | 0.11 |
| (2,2238) | 1:A:23:VAL:HG11 | 1:A:51:LEU:H | 10 | 0.11 |
| (2,2238) | 1:A:23:VAL:HG13 | 1:A:51:LEU:H | 10 | 0.11 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG23 | 9 | 0.11 |
| (2,2222) | 1:A:22:THR:HA | 1:A:22:THR:HG21 | 9 | 0.11 |
| (2,2209) | 1:A:21:VAL:HG12 | 1:A:19:ASP:H | 3 | 0.11 |
| (2,2209) | 1:A:21:VAL:HG11 | 1:A:19:ASP:H | 3 | 0.11 |
| (2,2209) | 1:A:21:VAL:HG13 | 1:A:19:ASP:H | 3 | 0.11 |
| (2,2196) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HD12 | 8 | 0.11 |
| (2,2196) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG22 | 8 | 0.11 |
| (2,2196) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG21 | 8 | 0.11 |
| (2,2196) | 1:A:19:ASP:HB2 | 2:B:132:ILE:HG23 | 8 | 0.11 |
| (2,2196) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HD12 | 8 | 0.11 |
| (2,2196) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HG21 | 8 | 0.11 |
| (2,2196) | 1:A:19:ASP:HB3 | 2:B:132:ILE:HG23 | 8 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD23 | 1:A:27:LYS:HE3 | 1 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD12 | 1:A:27:LYS:HE2 | 1 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD12 | 1:A:27:LYS:HE3 | 1 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD11 | 1:A:27:LYS:HE2 | 1 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD11 | 1:A:27:LYS:HE3 | 1 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD22 | 1:A:27:LYS:HE2 | 1 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD22 | 1:A:27:LYS:HE3 | 1 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD21 | 1:A:27:LYS:HE3 | 1 | 0.11 |
| (2,2166) | 1:A:16:LEU:HD23 | 1:A:27:LYS:HE2 | 1 | 0.11 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE2 | 5 | 0.11 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE1 | 5 | 0.11 |
| (2,2138) | 1:A:14:LEU:HG | 2:B:101:MET:HE3 | 5 | 0.11 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG2 | 8 | 0.11 |
| (2,1993) | 2:B:161:LYS:HE2 | 2:B:161:LYS:HG3 | 8 | 0.11 |
| (2,1993) | 2:B:161:LYS:HE3 | 2:B:161:LYS:HG3 | 8 | 0.11 |
| (2,1988) | 2:B:161:LYS:HD2 | 2:B:161:LYS:HA | 3 | 0.11 |
| (2,1988) | 2:B:161:LYS:HD3 | 2:B:161:LYS:HA | 3 | 0.11 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD13 | 7 | 0.11 |
| (2,1953) | 2:B:155:ILE:HA | 2:B:155:ILE:HD12 | 7 | 0.11 |
| (2,1934) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG3 | 3 | 0.11 |
| (2,1934) | 2:B:152:GLU:HB3 | 2:B:152:GLU:HG3 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1934) | 2:B:152:GLU:HB2 | 2:B:152:GLU:HG2 | 3 | 0.11 |
| (2,1876) | 2:B:143:ILE:HG21 | 2:B:147:ASN:HB2 | 5 | 0.11 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB2 | 5 | 0.11 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB3 | 5 | 0.11 |
| (2,1876) | 2:B:143:ILE:HG21 | 2:B:147:ASN:HB2 | 9 | 0.11 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB2 | 9 | 0.11 |
| (2,1876) | 2:B:143:ILE:HG22 | 2:B:147:ASN:HB3 | 9 | 0.11 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB2 | 9 | 0.11 |
| (2,1827) | 2:B:137:ASP:HA | 2:B:137:ASP:HB3 | 9 | 0.11 |
| (2,181) | 2:B:107:TYR:H | 2:B:146:LEU:HD12 | 4 | 0.11 |
| (2,181) | 2:B:107:TYR:H | 2:B:146:LEU:HD11 | 4 | 0.11 |
| (2,181) | 2:B:107:TYR:H | 2:B:146:LEU:HD13 | 4 | 0.11 |
| (2,181) | 2:B:107:TYR:H | 2:B:146:LEU:HD21 | 4 | 0.11 |
| (2,181) | 2:B:107:TYR:H | 2:B:146:LEU:HD23 | 4 | 0.11 |
| (2,1743) | 2:B:124:LYS:HG2 | 2:B:124:LYS:HE3 | 5 | 0.11 |
| (2,1743) | 2:B:124:LYS:HG3 | 2:B:124:LYS:HE3 | 5 | 0.11 |
| (2,1743) | 2:B:124:LYS:HG3 | 2:B:124:LYS:HE2 | 5 | 0.11 |
| (2,1728) | 2:B:123:ILE:HD13 | 2:B:139:LEU:HA | 4 | 0.11 |
| (2,1728) | 2:B:123:ILE:HD12 | 2:B:139:LEU:HA | 4 | 0.11 |
| (2,1728) | 2:B:123:ILE:HD12 | 2:B:108:LEU:HA | 4 | 0.11 |
| (2,1728) | 2:B:123:ILE:HD11 | 2:B:139:LEU:HA | 4 | 0.11 |
| (2,1722) | 2:B:122:ASP:HA | 2:B:122:ASP:HB2 | 7 | 0.11 |
| (2,1722) | 2:B:122:ASP:HA | 2:B:122:ASP:HB3 | 7 | 0.11 |
| (2,1721) | 2:B:122:ASP:HA | 2:B:125:LYS:HG2 | 1 | 0.11 |
| (2,1721) | 2:B:122:ASP:HA | 2:B:125:LYS:HG3 | 1 | 0.11 |
| (2,1681) | 2:B:118:PRO:HA | 2:B:122:ASP:HB3 | 2 | 0.11 |
| (2,1681) | 2:B:118:PRO:HA | 2:B:122:ASP:HB2 | 2 | 0.11 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG2 | 4 | 0.11 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG3 | 4 | 0.11 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG2 | 4 | 0.11 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG3 | 4 | 0.11 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG2 | 5 | 0.11 |
| (2,1629) | 2:B:105:ALA:HB2 | 2:B:101:MET:HG3 | 5 | 0.11 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG2 | 5 | 0.11 |
| (2,1629) | 2:B:105:ALA:HB3 | 2:B:101:MET:HG3 | 5 | 0.11 |
| (2,1614) | 2:B:101:MET:HE1 | 1:A:14:LEU:HB2 | 7 | 0.11 |
| (2,1614) | 2:B:101:MET:HE3 | 1:A:14:LEU:HB2 | 7 | 0.11 |
| (2,1614) | 2:B:101:MET:HE2 | 1:A:14:LEU:HB2 | 7 | 0.11 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG11 | 3 | 0.11 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG13 | 3 | 0.11 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG22 | 3 | 0.11 |
| (2,1605) | 1:A:63:VAL:HA | 1:A:63:VAL:HG23 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1542) | 1:A:51:LEU:HD22 | 1:A:56:ILE:HB | 1 | 0.11 |
| (2,1542) | 1:A:51:LEU:HD21 | 1:A:56:ILE:HB | 1 | 0.11 |
| (2,1542) | 1:A:51:LEU:HD23 | 1:A:56:ILE:HB | 1 | 0.11 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD12 | 9 | 0.11 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD11 | 9 | 0.11 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:51:LEU:HD13 | 9 | 0.11 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD12 | 9 | 0.11 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD11 | 9 | 0.11 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:46:LEU:HD13 | 9 | 0.11 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD21 | 9 | 0.11 |
| (2,1520) | 1:A:47:PHE:HA | 1:A:59:LEU:HD23 | 9 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG12 | 6 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG11 | 6 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG13 | 6 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG23 | 6 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG12 | 8 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG11 | 8 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG13 | 8 | 0.11 |
| (2,1494) | 1:A:41:PRO:HA | 1:A:39:VAL:HG23 | 8 | 0.11 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 4 | 0.11 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 4 | 0.11 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 4 | 0.11 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD2 | 6 | 0.11 |
| (2,1491) | 1:A:40:GLU:HG2 | 1:A:41:PRO:HD3 | 6 | 0.11 |
| (2,1491) | 1:A:40:GLU:HG3 | 1:A:41:PRO:HD3 | 6 | 0.11 |
| (2,1442) | 1:A:33:LYS:HA | 1:A:33:LYS:HG2 | 10 | 0.11 |
| (2,1442) | 1:A:33:LYS:HA | 1:A:33:LYS:HG3 | 10 | 0.11 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG12 | 9 | 0.11 |
| (2,1337) | 1:A:14:LEU:HG | 1:A:56:ILE:HG13 | 9 | 0.11 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG21 | 1 | 0.11 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG23 | 1 | 0.11 |
| (2,1321) | 1:A:7:LEU:HA | 1:A:10:ILE:HG22 | 1 | 0.11 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB3 | 10 | 0.11 |
| (2,130) | 1:A:48:ALA:H | 1:A:49:LYS:HB2 | 10 | 0.11 |
| (2,1285) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HB3 | 3 | 0.11 |
| (2,1285) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HB2 | 3 | 0.11 |
| (2,1285) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HB3 | 3 | 0.11 |
| (2,1285) | 1:A:4:VAL:HG12 | 1:A:7:LEU:HB3 | 3 | 0.11 |
| (2,1285) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HB3 | 3 | 0.11 |
| (2,1285) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HB2 | 3 | 0.11 |
| (2,1285) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HB3 | 3 | 0.11 |
| (2,1285) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HB2 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD22 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD21 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD23 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD22 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD21 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD23 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD22 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD21 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD23 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD22 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD21 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD23 | 3 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD22 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD21 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG11 | 1:A:7:LEU:HD23 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD22 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD21 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG22 | 1:A:7:LEU:HD23 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD22 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD21 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG21 | 1:A:7:LEU:HD23 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD22 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD21 | 7 | 0.11 |
| (2,1283) | 1:A:4:VAL:HG23 | 1:A:7:LEU:HD23 | 7 | 0.11 |
| (2,128) | 1:A:48:ALA:H | 1:A:28:ILE:HD12 | 1 | 0.11 |
| (2,128) | 1:A:48:ALA:H | 1:A:28:ILE:HD13 | 1 | 0.11 |
| (2,1225) | 2:B:162:LEU:HB2 | 2:B:162:LEU:HG | 3 | 0.11 |
| (2,1225) | 2:B:162:LEU:HB3 | 2:B:162:LEU:HG | 3 | 0.11 |
| (2,1225) | 2:B:162:LEU:HB2 | 2:B:162:LEU:HG | 5 | 0.11 |
| (2,1225) | 2:B:162:LEU:HB3 | 2:B:162:LEU:HG | 5 | 0.11 |
| (2,1225) | 2:B:162:LEU:HB2 | 2:B:162:LEU:HG | 9 | 0.11 |
| (2,1225) | 2:B:162:LEU:HB3 | 2:B:162:LEU:HG | 9 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 3 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 3 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 3 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 5 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 5 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 5 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG22 | 6 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG21 | 6 | 0.11 |
| (2,1217) | 2:B:159:ILE:HA | 2:B:159:ILE:HG23 | 6 | 0.11 |
| (2,12) | 1:A:3:SER:H | 1:A:6:GLU:HG2 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,12) | 1:A:3:SER:H | 1:A:6:GLU:HG3 | 5 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD11 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD22 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD21 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG12 | 2:B:146:LEU:HD23 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD11 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD22 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD21 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG11 | 2:B:146:LEU:HD23 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD22 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD21 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG13 | 2:B:146:LEU:HD23 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD11 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD13 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD22 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG22 | 2:B:146:LEU:HD23 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG21 | 2:B:146:LEU:HD23 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD11 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD13 | 7 | 0.11 |
| (2,1173) | 2:B:154:VAL:HG23 | 2:B:146:LEU:HD23 | 7 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 1 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 1 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 2 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 2 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 3 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 3 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 6 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 6 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD11 | 7 | 0.11 |
| (2,1153) | 2:B:151:ILE:HA | 2:B:151:ILE:HD13 | 7 | 0.11 |
| (2,1105) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD12 | 3 | 0.11 |
| (2,1105) | 2:B:143:ILE:HG23 | 2:B:143:ILE:HD13 | 3 | 0.11 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD12 | 3 | 0.11 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD11 | 3 | 0.11 |
| (2,1105) | 2:B:143:ILE:HG21 | 2:B:143:ILE:HD13 | 3 | 0.11 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG21 | 4 | 0.11 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG12 | 4 | 0.11 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG11 | 4 | 0.11 |
| (2,1085) | 2:B:142:VAL:HA | 2:B:142:VAL:HG22 | 4 | 0.11 |
| (1,94) | 2:B:145:GLU:H | 2:B:141:LYS:O | 10 | 0.11 |
| (1,82) | 2:B:129:SER:H | 2:B:125:LYS:O | 6 | 0.11 |
| (1,82) | 2:B:129:SER:H | 2:B:125:LYS:O | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|--------|---------------|---------------|----------|---------------|
| (1,75) | 2:B:126:ILE:N | 2:B:122:ASP:O | 6 | 0.11 |
| (1,73) | 2:B:125:LYS:N | 2:B:121:LYS:O | 9 | 0.11 |
| (1,6) | 1:A:9:CYS:H | 1:A:5:SER:O | 3 | 0.11 |
| (1,6) | 1:A:9:CYS:H | 1:A:5:SER:O | 5 | 0.11 |
| (1,56) | 2:B:107:TYR:H | 2:B:103:TYR:O | 1 | 0.11 |
| (1,55) | 2:B:107:TYR:N | 2:B:103:TYR:O | 7 | 0.11 |
| (1,47) | 1:A:48:ALA:N | 1:A:44:PRO:O | 9 | 0.11 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 3 | 0.11 |
| (1,46) | 1:A:47:PHE:H | 1:A:43:TRP:O | 9 | 0.11 |
| (1,45) | 1:A:47:PHE:N | 1:A:43:TRP:O | 2 | 0.11 |
| (1,42) | 1:A:45:GLY:H | 1:A:41:PRO:O | 10 | 0.11 |
| (1,31) | 1:A:31:LEU:N | 1:A:27:LYS:O | 5 | 0.11 |
| (1,19) | 1:A:16:LEU:N | 1:A:12:SER:O | 4 | 0.11 |
| (1,19) | 1:A:16:LEU:N | 1:A:12:SER:O | 7 | 0.11 |
| (1,13) | 1:A:13:ALA:N | 1:A:9:CYS:O | 2 | 0.11 |

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

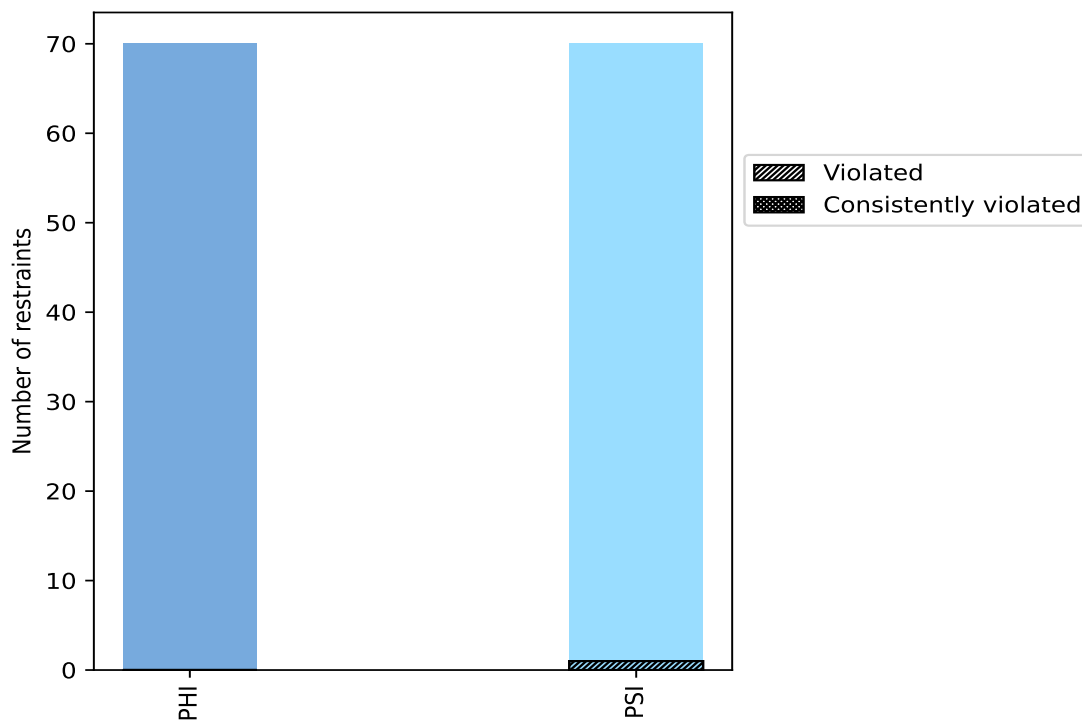
10.1 Summary of dihedral-angle violations [i](#)

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 | 70 | 50.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| PSI | 70 | 50.0 | 1 | 1.4 | 0.7 | 0 | 0.0 | 0.0 |
| Total | 140 | 100.0 | 1 | 0.7 | 0.7 | 0 | 0.0 | 0.0 |

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

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



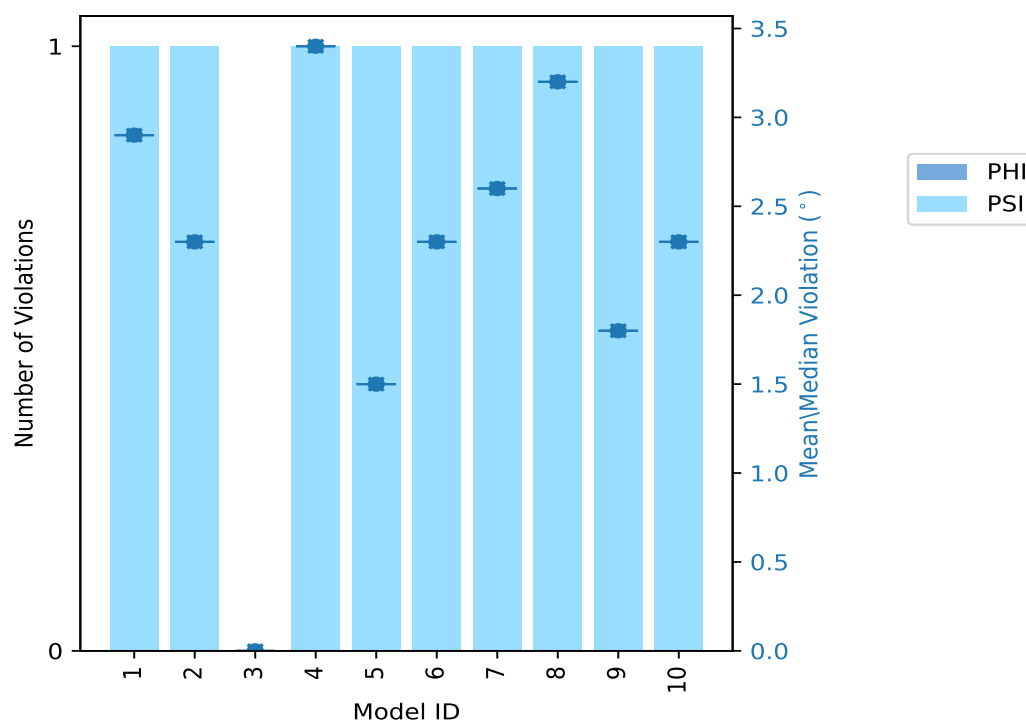
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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 | 0 | 1 | 1 | 2.9 | 2.9 | 0.0 | 2.9 |
| 2 | 0 | 1 | 1 | 2.3 | 2.3 | 0.0 | 2.3 |
| 3 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 4 | 0 | 1 | 1 | 3.4 | 3.4 | 0.0 | 3.4 |
| 5 | 0 | 1 | 1 | 1.5 | 1.5 | 0.0 | 1.5 |
| 6 | 0 | 1 | 1 | 2.3 | 2.3 | 0.0 | 2.3 |
| 7 | 0 | 1 | 1 | 2.6 | 2.6 | 0.0 | 2.6 |
| 8 | 0 | 1 | 1 | 3.2 | 3.2 | 0.0 | 3.2 |
| 9 | 0 | 1 | 1 | 1.8 | 1.8 | 0.0 | 1.8 |
| 10 | 0 | 1 | 1 | 2.3 | 2.3 | 0.0 | 2.3 |

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

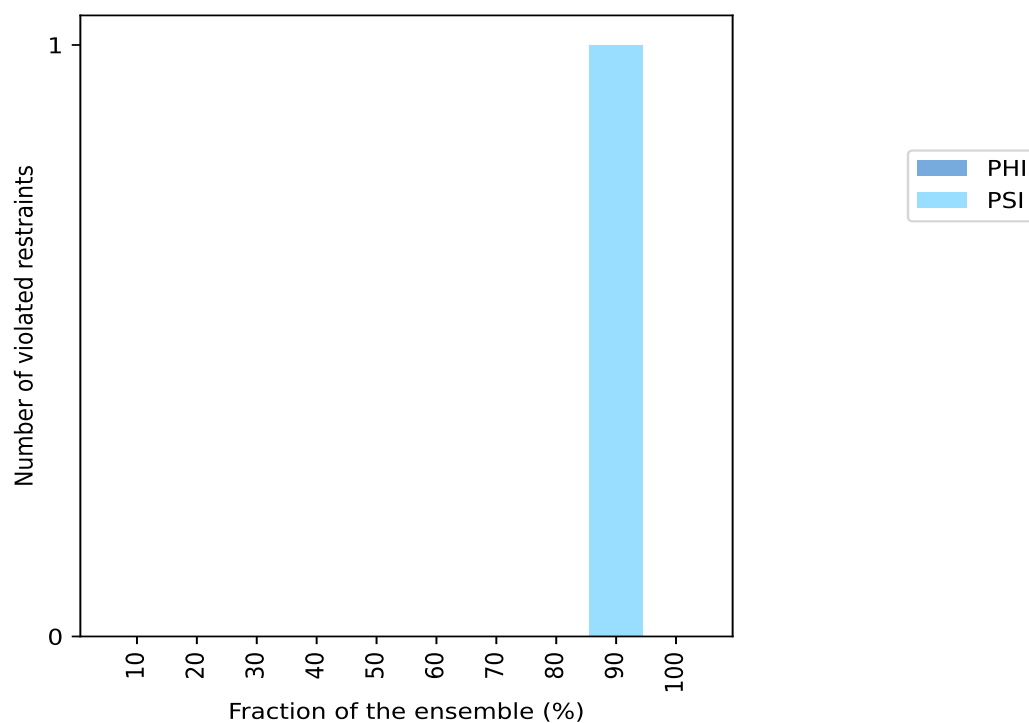
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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 | % |
| 0 | 0 | 0 | 1 | 10.0 |
| 0 | 0 | 0 | 2 | 20.0 |
| 0 | 0 | 0 | 3 | 30.0 |
| 0 | 0 | 0 | 4 | 40.0 |
| 0 | 0 | 0 | 5 | 50.0 |
| 0 | 0 | 0 | 6 | 60.0 |
| 0 | 0 | 0 | 7 | 70.0 |
| 0 | 0 | 0 | 8 | 80.0 |
| 0 | 1 | 1 | 9 | 90.0 |
| 0 | 0 | 0 | 10 | 100.0 |

¹ Number of models with violations

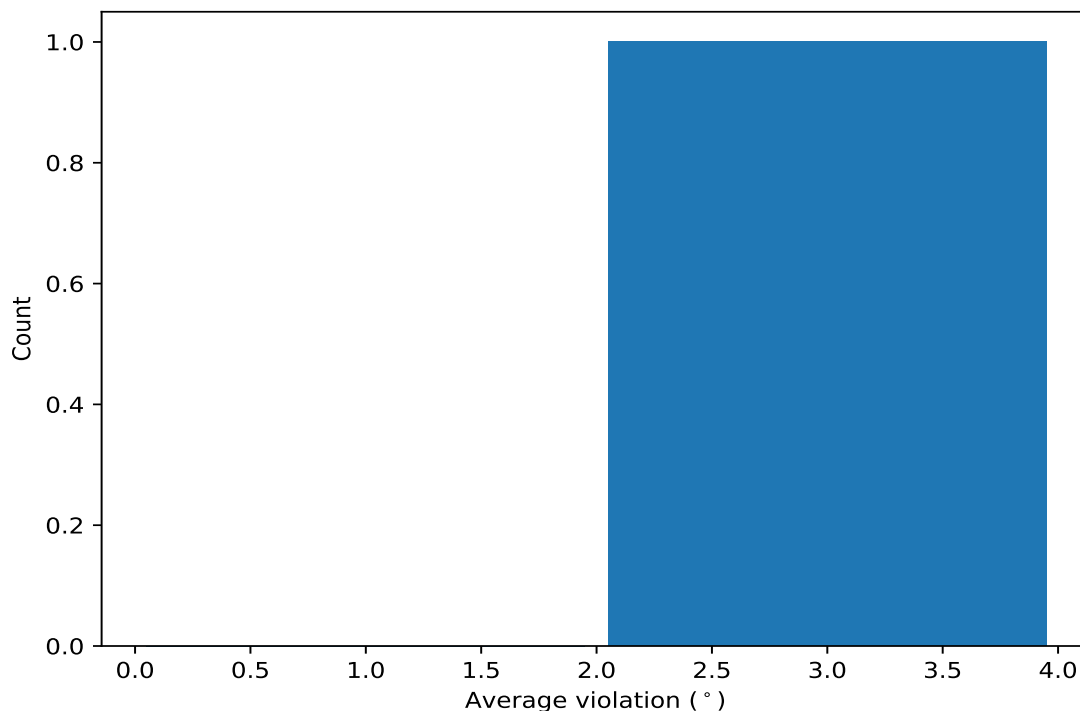
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

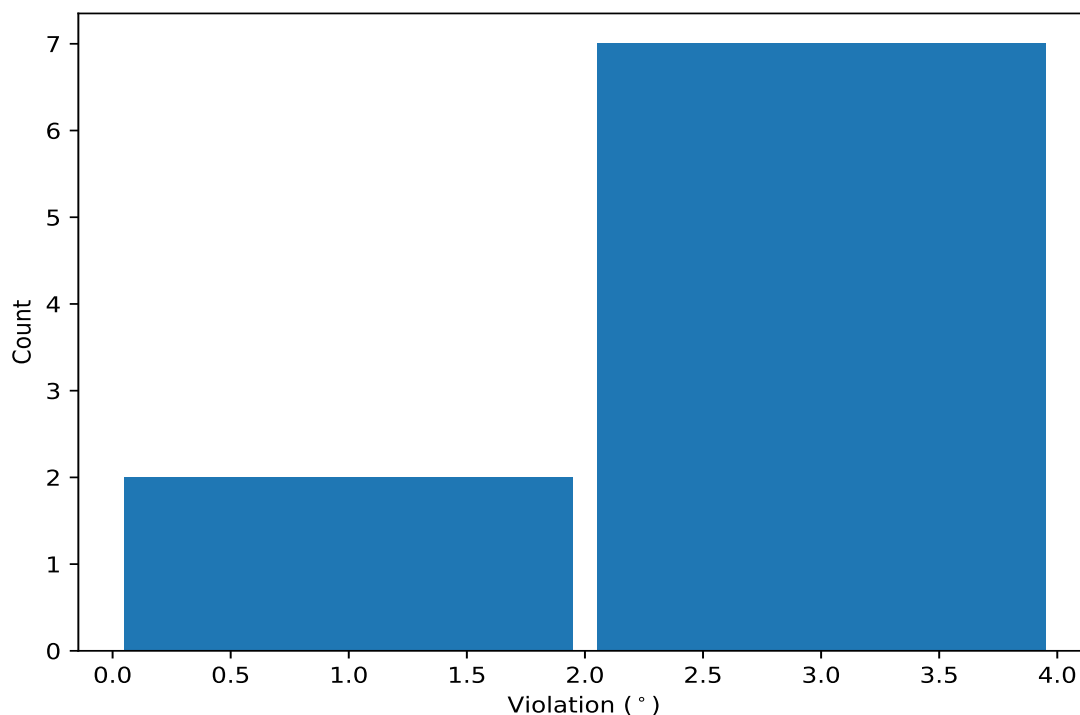
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 9 | 2.48 | 0.58 | 2.3 |

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 (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 4 | 3.4 |
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 8 | 3.2 |
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 1 | 2.9 |
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 7 | 2.6 |
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 2 | 2.3 |
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 6 | 2.3 |
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 10 | 2.3 |
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 9 | 1.8 |
| (1,138) | 2:B:158:GLY:N | 2:B:158:GLY:CA | 2:B:158:GLY:C | 2:B:159:ILE:N | 5 | 1.5 |